Curriculum Vitae

Name : **Kwang Soo Kim**

Born : Feb. 6, 1950 (Korea)

Address : (office) Department of Chemistry, School of Natural Science, Ulsan National Institute of Science and Technology (UNIST), (Bldg. 103) 50 UNIST-gil, Ulsan 44919, Korea
(home) UNIST Faculty Apt. 402-601, 50 UNIST-gil, Ulsan National Institute of Science and Technology, Ulsan, 44919, Korea

Tel : (+82) 52-217-5410; Cellphone: (+82-10-5067-2110). **Fax:** (+82) 52-217-5419

E-mail : kimks@unist.ac.kr

Web page: http://csm.unist.ac.kr (Center for Superfunctional Materials)
http://chemistry.unist.ac.kr/facultymembers (Chem, UNIST)
http://chemistry.unist.ac.kr/people/faculty-list/ (Chem, UNIST)
http://www.researcherid.com/rid/C-7538-2012 (ResearcherID)
https://publons.com/researcher/1333758/kwang-soo-kim/ (Publons)
http://orcid.org/0000-0002-6929-5359 (Orcid)
http://scholar.google.com/citations?hl=en&user=dWoR7zwAAAAJ (Google)
http://www.iaqms.org/members/kim.php (IQMS)

Education :

9/78-6/82	Univ. of California, Berkeley, Chemistry, Ph.D.
9/73-6/75	Korea Advanced Institute of Science & Tech., Physics, M.S.
3/71-2/73	Seoul National Univ., Applied Chemistry, M.Eng..
3/67-2/71	Seoul National Univ., Engineering College, Applied Chemistry, B.S.

Professional Experiences :

3/14-present	Ulsan National Institute of Science and Technology (UNIST), Center for Superfunctional Materials, Director
3/14-present	Ulsan National Institute of Science and Technology (UNIST), Dept. of Chemistry, School of Natural Science, Distinguished Professor.
12/97-2/14	Pohang Univ. of Science & Tech., Center for Superfunctional Materials, Director
1/88- 2/14	Pohang Univ. of Science & Tech., Dept. of Chemistry, Ass. - Full Professor.
8/04- 6/05	Columbia Univ. Dept. Elect. Engineering & NanoCenter, Visiting Scholar
8/94- 7/95	MIT, Dept. of Physics, Visiting Scientist
8/85-12/87	Rutgers Univ., Visiting Assistant Professor, Research Assistant Professor
9/82- 7/85	IBM/NFCR, Postdoctoral Research Fellow
9/75- 9/78	Chungnam National Univ. Dept. of Physics, Instructor, Assistant Professor

Professional Societies: Amer. Chem. Soc. (ACS), Korean Chem. Soc. (KCS),
Korean Academy of Science and Tech. [Fellow] (1999),
International Academy of Quantum Molecular Science (IAQMS) membership (2009):
http://www.iaqms.org/members/kim.php

Editors and Board Members of International Journals:

Wiley Interdisciplinary Reviews: Computational Molecular Science (Wiley); (2011-present)
Chemistry Letters (Chem. Soc. Japan); (2010- present)
Chemical Physics Letters (Elsevier); (2009- present)

Advances in Physical Chemistry (Hindawi); (2008- present)

Computational and Theoretical Chemistry (Elsevier); (2007- present)

Journal of Computational Chemistry (Wiley-VCH); (2005- present)

NPG Asia Materials (Nature Publishing Group); (2009-2018)

Chemistry – An Asian Journal (Wiley-VCH); (2006- 2013)

Bulletin of Korean Chemical Society; (2000- 2009) [Associate Editor, 3/00-12/03]

Journal of Physical Chemistry A, B, C (Am. Chem. Soc.); (2015-2017); Senior Editor

Board Member of International Conferences:

World Association of Theoretically Oriented Chemistry (WATOC) (2005- present)

Asian Pacific Conference on Theoretical and Computational Chemistry (APCTCC) (2005- present)

Research Interests: Theoretical/computational chemistry/physics (density functional theory, ab initio theory, molecular dynamics, statistical thermodynamics, transport phenomena, nonequilibrium thermodynamics, tensor network, deep machine learning, quantum computing)

Experimental Nanosciences (functional molecules/materials, molecular sensing, molecular engineering, nano electronic/spintronic/photonic devices, light harvesting, photosynthesis, green chemistry, energy materials, quantum dots, DNA sequencing, molecular robots)

Awards & Honors: Listed in Global highly cited researchers 2018 & 2019, Clarivate Analytics.
https://clarivate.com/blog/news/global-highly-cited-researchers-2018-list-reveals-influential-scientific-researchers-and-their-institutions/

Ranked 32nd in the world (H-index 92; cites: 48464) in Ranking of Nanotechnology & Nanoscience experts according to Google Scholar public profiles 2018:
http://www.webometrics.info/en/node/198 (Ranking Web of Universities).

CMOA Senior Scientist medal for outstanding scientific achievements at the Quantum Systems in Chemistry, Physics, and Biology (QSCP XXII) conference, China (2017)

Mulliken Lecture, Univ. of Georgia, USA (2011)

Fukui medal from Asia-Pacific Association of Theoretical and Computational Chemistry (APATCC) (2011): [http://www.apatcc.org/news.html]

Ranked within the top 500 chemists (only one among Korean nationals): H-index ranking of well known living chemists: Updated online by Chemistry World, UK, on Dec 12, 2011:
http://www.rsc.org/images/H-index%20ranking%20of%20living%20chemists(December%202011)_tcm18-211414.pdf

Korea Premium Science and Technology Award (2010) 대한민국 최고과학기술인상

Korea National Honor Scientist (2010) 국가과학자

International Academy of Quantum Molecular Science (IAQMS): membership elected (2009): [http://www.iaqms.org/members/kim.php]

UNIST Distinguished Professor (2014-present)

Postech Fellow (2009-2014)

Hongdeuk Chaired Professor (2004-2007)

Korea Science Award (2004) 한국과학상

Academic Achievement Award from the Korean Chemical Society (2001)

Invited Talks: ~130 invited talks in international conferences including **~35** plenary and keynote talks

Citations/Impact.: > **500** publications in SCI journals;

SCI Citations: ~50,000 (ISI), ~65,000 (Google); H-index: 90 (ISI), 100 (Google)

Brief Introduction of Publications:

- Over 500 papers have been published in prestigious journals such as Nature, Science, Nature Energy, Nature Nanotech., Nature Cataly., Nature Commun., Chem. Rev., Chem. Soc. Rev., Proc. Natl. Acad. Sci., Acc. Chem. Res., Phys. Rev. X, Phys. Rev. Lett, J. Am. Chem. Soc., Angew. Chem. Int. Ed., Chem. Sci., Chem. Comm., Chem. Eur. J., Org. Lett., J. Org. Chem., Phys. Rev., Appl. Phys. Lett., J. Chem. Phys., J. Phys. Chem., Nano Lett., ACS Nano, ACS Energy Lett., ACS Catal., Adv. Mater., Adv. Energy Mater., Adv. Funct. Mater., J. Mater. Chem. A, etc. (refer to: http://csm.unist.ac.kr). One book and twelve book chapters have been published [Marcel Dekker, Elsevier, American Science, World Scientific., etc..

- These papers have been well cited. Organic nanotubes and nanowires (*JACS* 2001, *Science* 2001) and left handed helices (*JACS* 2001) were featured in *C&EN*. Extraction of thinnest carbon nanotubes (*PNAS* 2005) was featured in *Nature* (Materials website). Supermagnetism in graphene nanoribbon (*Nature Nanotech.* 2008) was featured in NPG Asia materials. Large scale graphene ultrathin films (*Nature* 2009a) which we collaborated with my former student (BH Hong) was featured in *New York Times* and cited in the official "Nobelprize.org" press release for the 2010 Nobel prize in physics. Near field focusing and magnification beyond the diffraction limit of the self assembled nanolenses was published (*Nature* 2009b), which was featured in *Laser Focus World*, *Nature Nanotech., NPG Asia Materials (Nature Publ. Group)*, *Technology Review (MIT), Chem. & Eng. News (Am. Chem. Soc.)*, *Nanotechweb.org (IOP),* and Korean television and newspapers. An ultrafast DNA sequencing method (*Nature Nanotech.* 2011) was featured in *NPG Asia Materials (Nature Publ. Group),* magzines, newspapers and TV. Synthesis of 3rd type of Calix compounds (*Nature Commun.* 2013a) and highly active Pt-DNA-graphene catalysts for fuel cell (*Nature Commun.*2013b) were featured in newspapers. Synthesis of superior electrocatalysts (*Nature Energy, 2018) were featured in newspapers and TV.*

Brief Summary of SCI Publications

Journals (IF): No. of publications: [Total: 527]

Nature	**(43.070): 2,**	**Science**	**(41.037): 1,**	**Nature Energy**	**(54.000): 1,**
Nature Nanotech.	**(33.407): 3,**	**Nature Catal.**	**(-): 1,**	**Nature Commun.**	**(11.878): 5,**
Chem. Rev.	**(54.301): 3,**	**Chem. Soc. Rev.**	**(40.443): 2,**	**Adv. Mater.**	**(25.809):10,**
Adv. Ener. Mater.	**(24.884):4,**	**Prog. Mater. Sci.**	**(23.725):1,**	**Acc. Chem. Res.**	**(21.661): 2,**
ACS Ener. Lett.	**(16.331): 2,**	**Adv. Funct. Mater.**	**(15.621): 4,**	**Nano Energy**	**(15.548): 2,**
J. Am. Chem. Soc.	**(14.695):29,**	**ACS Nano**	**(13.903):19,**	**Nano Lett.**	**(12.279): 4,**
Angew.Chem.Int.Ed.	**(12.257):6,**	**Phys. Rev. X**	**(12.211): 1,**	**ACS Catal.**	**(12.211): 1,**
J. Mater. Chem. A	**(10.733):14,**	**Chem. Mater.**	**(10.159): 1,**	**Proc.Nat.Acad.Sci.**	**(9.580): 5,**
Chem. Sci.	**(9.556): 1,**	**Phys. Rev. Lett.**	**(9.227): 9,**	**ACS Appl.Mater.Inter.**	**(8.456):7,**
J. Hazard Mater.	**(7.650):1,**	**J. Power Source**	**(7.467): 1,**	**Carbon**	**(7.466): 4,**
J. Phys. Chem. Lett.	**(7.329): 6**	**Env. Sci. Tech.**	**(7.149):1,**	**Nanoscale**	**(6.970): 8,**
ACS Sensors	**(6.944): 1,**	**Org. Lett.**	**(6.555):13,**	**Anal. Chem.**	**(6.350):1,**
Chem. Commun.	**(6.164):9,**	**J.Chem.Theor.Comput.**	**(5.313):19,**	**Chem. Eur. J.**	**(5.160):13,**

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Inorg. Chem.	**(4.850): 1,**	**J. Org. Chem.**	**(4.745):11,**	**J. Phys.Chem. C**	**(4.309): 12,**
J. Ind. Eng. Chem.	**(4.978): 1,**	**Dyes & Pigments**	**(4.018): 1,**	**Sci. Rep.**	**(4.011): 4,**
Opt. Lett.	**(3.866): 1**	**J. Struct. Biol**	**(3.754):1,**	**Phys. Rev. B**	**(3.736): 27,**
Chem. Asian J.	**(3.698): 2,**	**Phys.Chem.Chem.Phys.**	**(3.567):14,**	**Opt. Exp.**	**(3.561): 2,**
Appl. Phys. Lett.	**(3.521): 4,**	**Org. Biomol. Chem.**	**(3.490);3.**	**Nanotechnology**	**(3.399): 9,**
CrystEngComm	**(3.382):2,**	**J. Comput. Chem.**	**(3.194):9,**	**ChemPhysChem**	**(3.077); 1,**
RSC Adv.	**(3.049): 4,**	**J. Chem. Phys.**	**(2.997):85,**	**J. Phys. Chem. B**	**(2.923):14,**
Phys. Rev. A	**(2.907): 3,**	**Comput. Mater. Sci.**	**(2.644) 1,**	**J. Phys. Chem. A**	**(2.641):31,**
Bioorg.Med.Chem.Lett.	**(2.448):1,**	**Tetrahedron**	**(2.379); 2,**	**Phys. Rev. E**	**(2.353): 3,**

Pure Appl. Chem.	**(2.350);1,**	**Int. J. Quant. Chem.**	**(2.263): 2,**	**Tetrahedron Lett.**	**(2.259); 1,**
Struct. Chem.	**(2.178); 1,**	**J. Mol. Struct.**	**(2.120); 1,**	**Curr. Appl. Phys.**	**(2.010): 1,**
J. Chem. Phys. Lett.	**(1.901):10,**	**Mol. Graph. Model.**	**(1.863):2,**	**Theor. Chem. Acc.**	**(1.598); 2,**
Mol. Phys.	**(1.571): 6,**	**J. Phys. Org. Chem.**	**(1.530): 1,**	**J. Math. Phys.**	**(1.355): 1,**

Selected Papers:

[1] ***Nature*** 460, 498 (2009). [IF: 43.070; Corresponding Author; No. of citations: ~**250**].
Near-field focusing and magnification through self-assembled nanoscale spherical lenses,
J. Y. Lee, B. H. Hong, W. Y. Kim, S. K. Min, Y. Kim, M. V. Jouravlev, R. Bose, K. S. Kim, I.-C. Hwang, L. J. Kaufman, C. W. Wong, P. Kim, and K. S. Kim
Featured in *Laser Focus World*, *NPG Asia Materials (Nature Publ. Group)*, *Technology Review (MIT), Chem. & Eng. News (Am. Chem. Soc.)*, *Nanotechweb.org(IOP),*and Korean television and newspapers

[2] ***Nature Nanotechnol***. 3, 408 (2008). [IF: 33.407; Corresponding Author; No. of citations: ~**600**].
Prediction of very large values of magnetoresistance in a graphene nanoribbon device,
W. Y. Kim and K. S. Kim
Featured in *NPG Asia Materials (Nature Publ. Group)* and Korean newspapers

[3] ***Nature Nanotechnol***. 6, 162 (2011). [IF: 33.407; Corresponding Author; No. of citations: ~**350**].
Fast DNA sequencing with a graphene-based nanochannel device,
S. K. Min, W. Y. Kim, Y. Cho, K. S. Kim
Featured in *NPG Asia Materials (Nature Publ .Group).* science news magazines, television and newspapers.

[4] ***Nature Energy*** 3, 773 (2018). [IF: 54.000; Corresponding Author; No. of Citations: ~**50**].
Multicomponent electrocatalyst with ultralow Pt loading and high hydrogen evolution activity,
J. N. Tiwari, S. Sultan, C. W. Myung, T. Yoon, N. Li, M. Ha, A. M. Harzandi, H. J. Park, D. Y. Kim, S. S. Chandrasekaran, W. G. Lee, V. Vij, H. Kang, T. J. Shin, H. S. Shin, G. Lee, Z. Lee, K. S. Kim

[5] ***Science*** 294, 348 (2001). [IF: 41.037; Corresponding Author; No. of Citations ~**600**].
Ultrathin Single-crystalline Silver Nanowire Arrays Formed in an Ambient Solution Phase,
B.H. Hong , S.C. Bae, C.-W. Lee, S. Jeong, and K.S. Kim
Featured in *Science and Chem.& Eng. News (Am. Chem. Soc.).*

[6] ***Nature*** 457, 706 (2009). [IF: 43.070, coauthor; No. of Citations: ~**7,200**]
Large-scale pattern growth of graphene films for stretchable transparent electrodes,
K. S. Kim, Y. Zhao, H. Jang, S. Y. Lee, J. M. Kim, K. S. Kim, J.-H. Ahn, P. Kim, J.-Y. Choi, and B. H. Hong
Featured in *New York Times, Chem. & Eng. News (Am. Chem. Soc.)*, *Nanotechweb.org(IOP), etc.*; cited in the official "Nobelprize.org" press release for the 2010 Nobel prize in physics.

[7] ***Nature Nanotechnol***. 5, 574 (2010). [IF: 33.407; coauthor; No. of Citations: ~**5,300**].
Roll-to-roll production of 30-inch graphene films for transparent electrodes,
S. Bae, H. Kim, Y. Lee, X. Xu, J.-S. Park, Y. Zheng, J. Balakrishnan, T. Lei, H. R. Kim, Y. I. Song, Y.-J. Kim, K. S. Kim, B. Ozyilmaz, J.-H. Ahn, B. H. Hong and S. Iijima
Featured in leading science magazines, Korean television and newspapers

[8] ***Nature Commun.*** 4, 2221 (2013) [IF: 11.878; Corresponding Author; No. of Citations: ~**120**].
Stable Pt nanoclusters on genomic DNA-graphene oxide with a high oxygen reduction reaction activity.
J. N. Tiwari, K. Nath, S. Kumar, R. N. Tiwari, K.C. Kemp, N. H. Le, D. H. Youn, J. S. Lee, K. S. Kim

[9] ***Nature Commun.*** 10, 5195 (2019) [IF: 11.878; Corresponding Author]
S. Sultan, M. Ha, D. Y. Kim, J. N. Tiwari, C. W. Myung, A. Meena, T. J. Shin, K. H. Chae, K. S. Kim, Superb water splitting activity of the electrocatalyst $Fe_3Co(PO_4)_4$ designed with computation aid. **Nat. Commun.** DOI : 10.1038/s41467-019-13050-3

[10] ***Nature Commun.*** 4, 1797 (2013) [IF: 11.878; Corresponding Author; No. of Citations: ~**60**].
Calix[n]imidazolium as a new class of positively charged homocalix compounds,
Y. Chun, N. J. Singh, I.-C. Hwang, J. W. Lee, S. U. Yu, and K. S. Kim

[11] ***Nature Catal.*** V. K. Singh, C. Yu, S. Badgujar, Y. Kim, Y. Kwon, D. Kim, J. Lee, T. Akhter, G. Thangavel, L. S. Park, J. Lee, P. C. Nandajan, R. Wannemacher, B. Milián-Medina, L. Lüer, K. S. Kim*, J. Gierschner*, M. S. Kwon* Highly efficient organic photocatalysts discovered via a computer-aided-design strategy for visible-light-driven atom transfer radical polymerization, Nature Catal. 1, 794-804 (2018).

[12] ***Nature Commun.*** 7, 13115 (2016). [IF: 11.878; Co-Corresponding Author; No. of Citations: ~**40**].
Structure-mechanism-based engineering of chemical regulators targeting distinct pathological factors in Alzheimer's disease, M. Beck , J. Derrick , R. Kerr , S. B. Oh , W. J. Cho , S. J. Lee , Y. Ji , J. Han, Z. Tehrani, N. Suh, S. Kim, S. Larsen, K. S. Kim, J.-Y. Lee, B. Ruotolo, M. H. Lim.

[13] ***Chem. Rev***. 112, 6156 (2012). [IF: 54.301; Corresponding Author; No. of Citations: ~**2100]**.
Functionalization of Graphene: Covalent and noncovalent approaches, derivatives and applications,
V. Georgakilas, M. Otyepka, A. B. Bourlinos, V. Chandra, N. Kim, K. C. Kemp, P. Hobza, R. Zboril, and K. S. Kim

[14] ***Chem. Rev***. 100, 4145 (2000). [IF: 54.301; Corresponding Author; No. of Citations: ~**900**].
Molecular Clusters of π-Systems: Theoretical Studies of Structures, Spectra and Origin of Interaction Energies,
K. S. Kim, P. Tarakeshwar, J. Y. Lee

[15] ***Chem. Rev.*** 116, 5464 (2016). [IF: 54.301; Co-Corresponding Author; No. of Citations: ~**700**].
Non-Covalent Functionalization of Graphene and Graphene Oxide for Energy Materials, Biosensing, Catalytic, and Biomedical Applications, V. Georgakilas, J. Tiwari, K. C., Kemp, J. Perman, A. Bourlinos, K. S. Kim, R. Zboril.
[16] ***Chem. Soc. Rev.*** 35, 355 (2006). [IF: 40.443; Corresponding Author; No. of Citations: ~**700**].
Imidazolium Receptors for the Recognition of Anions, J. Yoon, S. K. Kim, N. J. Singh and K. S. Kim
[17] ***ACS Nano*** 4, 3979 (2010). [IF: 13.709; Corresponding Author; No. of Citations: ~**1300**].
Water Dispersible Magnetite-Reduced Graphene Oxide Composites for Arsenic Removal,
V. Chandra, J. Park, Y. Chun, J. W. Lee, I.-C. Hwang, K. S. Kim
Featured in many science news magazines, television and newspapers.
[18] ***Proc. Nat. Acad. Sci.*** 112, 14156 (2015). [IF: 9.580; Corresponding Author].
High Temperature in-situ Crystallographic Observation of Reversible Gas Sorption in Impermeable Organic Cages. S. B. Baek, D. Moon, R. Graf, W. J. Cho, S. W. Park, T.-U. Yoon, S. J. Cho, I.-C. Hwang, Y.-S. Bae, H. W. Spiess, H. C. Lee, K. S. Kim.
[19] ***ACS Nano*** 8, 1827 (2014). [IF: 13.709; Corresponding Author; No. of Citations: ~**50**].
Two Dimensional Molecular Electronics Spectroscopy for Molecular Fingerprinting, DNA Sequencing and Cancerous DNA Recognition,
A. C. Rajan, M. R. Rezapour, J. Yun, Y. Cho, W. J. Cho, S. K. Min, G. Lee, and K. S. Kim
[20] ***Phys. Rev. Lett.*** 112, 157802 (2014) [IF: 9.227; Corresponding Author].
Limit of metastability for liquid and vapor phases of water,
W. J. Cho, J. Kim, J. Lee, T. Keyes, J. E. Straub, K. S. Kim.
[21] ***J. Am. Chem. Soc.*** 123, 10748 (2001) [IF: 14.695; Corresponding Author; No. of Citations: ~**250**].
Self-Assembled Arrays of Organic Nanotubes with Infinitely Long One-Dimensional H-Bond chains,
B. H. Hong, J. Y. Lee, C.-W. Lee, J. C. Kim, S. C. Bae, and K. S. Kim
[22] S. Sultan, J. N. Tiwari, A. N. Singh, S. Zhumagali, M. Ha, C. W. Myung, P. Thangavel, K. S. Kim, Single Atoms and Clusters Based Nano-Materials for Hydrogen Evolution, Oxygen Evolution Reactions, and full Water Splitting, Adv. Ener. Mater. 9, 1900624 (2019). DOI: 10.1002/aenm.201900624
[23] J. N. Tiwari, A. M. Harzandi, M. Ha, S. Sultan, C. W. Myung, H. J. Park, D. Y. Kim, P. Thangavel, A. N. Singh, P. Sharma, S. S. Chandrasekaran, F. Salehnia, J-W. Jang, H. S. Shin, Z. Lee, K. S. Kim, High-performance hydrogen evolution by Ru single-atoms and nitrided-Ru nanoparticles implanted on N-doped graphitic sheet, Adv. Ener. Mater. 9, 1900931 (2019). (cover).
[25] S. Sultan, J. N. Tiwari, J.-H. Jang, A. M. Harzandi, F. Salehnia, S. J. Yoo, K. S. Kim, Highly Efficient Oxygen Reduction Reaction Activity of Graphitic Tube Encapsulating Nitrided Co_xFe_y Alloy. Adv. Ener. Mater. 8, 1801002 (2018). DOI: 10.1002/aenm.201801002 (Back cover).
[26] C. W. Myung, S. Javaid, K. S. Kim, G. Lee, Rashba-Dresselhaus Effect in Inorganic/Organic Lead Iodide Perovskite Interfaces, ACS Energy Lett. 3, 1294-1300 (2018).
[27] C. W. Myung, J. Yun, G. Lee, K. S. Kim, A New Perspective on the Role of A-site Cations in Perovskite Solar Cells, Adv. Ener. Mater. 8, 1702898 (2018). DOI: 10.1002/aenm.201702898 (Back Cover).
[28] Seong Uk Yu, Hwiwon Lee, Woo Jong Cho, Chulhyun Kim, Moon Cheol Kang, Hyun-Joon Shin,
Namdong Kim, Sei Kwang Hahn, Kwang S. Kim, Spectromicroscopic Observation of a Live Single Cell in a Biocompatible Liquid-Enclosing Graphene System, Nanoscale, 10, 150-157 (2018).
DOI: 10.1039/C7NR05223E (Back Cover).
[29] T. Yoon, K. S. Kim, One step synthesis of CoS-doped β-Co(OH)2@amorphous MoS_2+x hybrid catalyst grown on nickel foam for high performance electrochemical overall water splitting, Adv. Funct. Mater. 41, 7386-7393 (2016).
[30] ***J. Phys. Chem. Lett.*** 7, 2478 (2016). [IF: 7.329; Corresponding Author.].
Electron Transport in Graphene Nanoribbon Field-Effect Transistor under Bias and Gate Voltages: Iso-Chemical Potential Approach, J. Yun, G. Lee, K. S. Kim.
[31] ***ACS Nano*** 11, 742 (2017). [IF: 13.709; Corresponding Author; No. of Citations: ~**20**].
Accelerated Bone-Regeneration by Two Photon Photoactivated Carbon Nitride Nanosheets, Tiwari, J. N.; Seo, Y.-K. ; Yoon, T.; Lee, W. G.; Cho, W. J.; Yousuf, M.; Harzandi, A. M. ; Kang, D.-S.; Kim, K.-Y.; Suh, P.-G.; Kim, K. S.
[32] ***J. Phys. Chem. A*** 111, 3446 (2007). [Corresponding Author; No. of Citations: ~**500**].
Understanding of Assembly Phenomena by Aromatic-aromatic interactions: benzene dimer and the substituted systems, E. C. Lee, D. Kim, P. Jurečka, P. Tarakeshwar, P. Hobza, and K. S. Kim.
[33] ***J. Am. Chem. Soc.*** 131, 15528 (2009). [IF: 14.695; Corresponding Author; No. of Citations: ~**400**].
Unique Sandwich Stacking of Pyrene-Adenine-Pyrene for Selective and Ratiometric Fluorescent Sensing of ATP at Physiological pH, Z. Xu, N. J. Singh, J. Lim, J. Pan, H. N. Kim, S. Park, K. S. Kim, and J. Yoon.
[34] ***Chem. Phys. Lett.*** 131, 451 (1986). [First Author; No. of Citations: ~**300**].

Revisiting small clusters of water molecules", K.S. Kim, M. Dupuis, G.C. Lie, and E. Clementi.

[35] ***J. Chem. Phys.*** 109, 5886 (1998). [Corresponding Author; No. of Citations: ~**300**].
Structures, binding energies, and spectra of isoenergetic water hexamer clusters: Extensive ab initio studies, J. Kim, K. S. Kim.

[36] ***J. Chem. Phys.*** 112, 9759 (2000). Error: 114, 3343 (2001). [Corresponding Author; No. of Citations: ~**300**].
Structures, energies, vibrational spectra, and electronic properties of water monomer to decamer, H. M. Lee, S. B. Suh, J. Y. Lee, P. Tarakeshwar, and K. S. Kim.

[37] ***J. Chem. Phys.*** 97, 6649 (1992). [Corresponding Author; No. of Citations: ~**260**].
Ab Initio Studies of the Water Dimer Using Large Basis Sets: The Structure and Thermodynamic Energies, K.S. Kim, B.J. Mhin, U-S. Choi, and K. Lee.

[38] ***J. Am. Chem. Soc.*** 116, 7399 (1994). [IF: 14.695; Corresponding Author; No. of Citations: ~**260**].
On Binding Forces between Aromatic Ring and Quaternary Ammonium Compound, K.S. Kim, J.Y. Lee, S.J. Lee, T.-K. Ha, and D.H. Kim.

[39] ***Org. Lett.*** 4, 2897 (2002). [Corresponding Author; No. of Citations: ~**250**].
Tripodal Nitro-Imidazolium Receptor for Anion Binding Driven by (C-H)+---X- Hydrogen Bonds, H. Ihm, S. Yun, H. G. Kim, J. K. Kim, and K. S. Kim.

[40] ***J. Am. Chem. Soc.*** 126, 8892 (2004). [IF: 114.695; Co-Corresponding Author; No. of Citations: ~**250**].
Fluorescent GTP-sensing in Aqueous Solution of Physiological pH, J. Y. Kwon, N. J. Singh, N. H. Kim, S. K. Kim, K. S. Kim, and J. Yoon.

[41] ***J. Phys. Chem. B*** 107, 9994 (2003). [Corresponding Author; No. of Citations: ~**230**].
Geometrical and electronic structures of gold, silver, and gold-silver binary clusters: Origins of ductility of gold and gold-silver alloy formation, H. M. Lee, M. Ge, B. R. Sahu, P. Tarakeshwar, and K. S. Kim.

[42] ***J. Chem. Phys.*** 113, 5259 (2000). [Corresponding Author; No. of Citations: ~**210**].
Comparative ab initio study of the structures, energetics and spectra of X-(H2O)n=1-4[X=F, Cl, Br, I] clusters, J. Kim, H.M. Lee, S.B. Suh, D. Majumdar, and K.S. Kim.

[43] ***Chem. Commun.*** 47, 3942 (2011). [Corresponding Author; No. of Citations: ~**300**].
Highly Selective Adsorption of Hg2+ by Polypyrrole-Reduced Graphene Oxide Composite, V. Chandra and K. S. Kim.

[44] ***Angew. Chem. Int. Ed.*** 44, 2899 (2005); Angew. Chem. 117, 2959 (2005).
[IF: 12.102; Corresponding Author; No. of Citations: ~**210**].
A Calix[4]imidazolium[2]pyridine as an Anion Receptor,
K. Chellappan, N. J. Singh, I.-C. Hwang, J. W. Lee, and K. S. Kim.

[45] ***J. Phys. Chem. A*** 108, 1250 (2004). [Corresponding Author; No. of Citations: ~**200**].
Theoretical investigations of anion-π interactions: The role of anions and the nature of π systems, D. Kim, P. Tarakeshwar, and K. S. Kim.

[46] ***J. Phys. Chem. A*** 107, 1228 (2003). [Corresponding Author; No. of Citations: ~**200**].
Cation-π Interactions: A Theoretical Investigation of the Interaction of Metallic and Organic Cations with Alkenes, Arenes, and Heteroarenes, D. Kim, S. Hu, P. Tarakeshwar, K. S. Kim, and J. M. Lisy.

[47] ***J. Am. Chem. Soc.*** 123, 3323 (2001). [IF: 14.357; Corresponding Author; No. of Citations: ~**180**].
Olefinic vs. aromatic pi-H interaction: A theoretical investigation of the nature of interaction of first-row hydrides with ethene and benzene, P. Tarakeshwar, H. S. Choi, and K. S. Kim.

[48] ***J. Chem. Phys.*** 102, 839 (1995). [Corresponding Author; No. of Citations: ~**180**].
Structures, Energetics, and Spectra of aqua-sodium(I): Thermodynamic Effects and Nonaddtive Interactions, J. Kim, S. Lee, S.J. Cho, B.J. Mhin, and K.S. Kim.

[49] ***J. Chem. Theor. Comput.*** 5, 515 (2009). [Corresponding Author; No. of Citations: ~**200**].
Comprehensive Energy Analysis for Various Types of pi-Interaction,
N. J. Singh, S. K. Min, D. Y. Kim, and K. S. Kim.

[50] ***Chem. Phys. Lett.*** 131, 451 (1986). [First Author; No. of Citations: ~**300**].
Revisiting small clusters of water molecules", K.S. Kim, M. Dupuis, G.C. Lie, and E. Clementi,

[51] ***ACS Nano***, 11, 3207-3212 (2017). [IF: 13.903] Two-Dimensional Excitonic Photoluminescence in Graphene on a Cu Surface. Y. Park, Y. Kim, C. W. Myung, R. A. Taylor, C. C. S. Chan, B. P. L. Reid, T. J. Puchtler, R. J. Nicholas, L. T. Singh, G. Lee, C.-C. Hwang, C.-Y. Park, and K. S. Kim.

[52] ***ACS Nano***, 10, 46-80 (2016). [IF: 13.903; Corresponding Author; No. of Citations: ~**200**]
Engineered Carbon-Nanomaterial Based Electrochemical Sensors for Biomolecules, J. N. Tiwari, V. Vij, K. C. Kemp, K. S. Kim.
[53] ***Acc. Chem. Res.*** 43, 111-120 (2010). [IF: 21.661; Corresponding Author; No. of Citations: ~**110**]
Tuning Molecular Orbitals in Molecular Electronics and Spintronics, W. Y. Kim and K. S. Kim.
[54] ***ACS Catal***. 7, 7196-7225 (2017). [IF: 12.211; Corresponding Author; No. of Citations: ~**200**]
Nickel–Based Electrocatalysts for Energy Related Applications: Oxygen Reduction, Oxygen Evolution, and Hydrogen Evolution Reactions, V. Vij, S. Sultan, A. M. Harzandi, A. Meena, J. N. Tiwari, W. -G. Lee, T. Yoon, K. S. Kim.

List of (SCI) Publications

http://csm.unist.ac.kr (Center),
http://www.researcherid.com/rid/C-7538-2012 (ResearcherID)
https://publons.com/researcher/1333758/kwang-soo-kim/ (Publons)
http://orcid.org/0000-0002-6929-5359
http://scholar.google.com/citations?hl=en&user=dWoR7zwAAAAJ

1. C. Hyun, J. H. Kim, J.-Y. Lee, G.-H. Lee, K. S. Kim, Atomic Scale Study for Black Phosphorus Degradation, RSC Adv. 10, 350 (2020).
2. Y. Kim, G. Lee, N. Li, J. Seo, K. S. Kim, N. Kim, Signature of multilayer growth of 2D Layered Bi2Se3 through heteroatom-assisted step-edge barrier reduction. npj 2D materials, 3, 51 (2019). https://doi.org/10.1038/s41699-019-0134-2
3. S. Sultan, M. Ha, D. Y. Kim, J. N. Tiwari, C. W. Myung, A. Meena, T. J. Shin, K. H. Chae, K. S. Kim, Superb water splitting activity of the electrocatalyst $Fe_3Co(PO_4)_4$ designed with computation aid. **Nature Commun.** 10, 5195 (2019). DOI : 10.1038/s41467-019-13050-3
4. Atanu Jana, Shynggys Zhumagali, Qiankai Ba, Arun S. Nissimagoudar and Kwang S. Kim*, Direct emission from quartet excited states triggered by upconversion phenomena in solid-phase synthesized fluorescent lead-free organic-inorganic hybrid compounds. J. Mater. Chem. A 7, 26504-26512 (2019). c9ta08268a.
5. Wang-Geun Lee, a Tae-Ung Yoon,b Youn-Sang Bae, Kwang S. Kim and Seung Bin Baek, Selective separation of Xe/Kr and adsorption of water in a microporous hydrogen-bonded organic framework. RSC Adv. 9, 36808-36814 (2019).
6. A. Jana, Q. Ba, A. S. Nissimagoudar, K. S. Kim, Formation of photoactive quasi-2D formamidinium lead iodide perovskite in water. J. Mater. Chem. A, 7, 25785-25790 (2019). DOI: 10.1039/C9TA09631K.
7. D. C. Yang, D. Y. Kim, K. S. Kim, Quantum Monte Carlo Study of the Water Dimer Binding Energy and Halogen−π Interactions, J. Phys. Chem. A 123, 7785−7791 (2019).
8. S. Kajal, G.H. Kim, C. W. Myung, Y. S. Shin, J. Kim, J. Jeong, A. Jana, J. Y. Kim, K. S. Kim, A thermally stable, barium stabilized α-CsPbI3 perovskite for optoelectronic devices, J. Mater. Chem. A. 7, 21740 (2019). DOI: 10.1039/C9TA07827D
9. Q. Ba, A. Jana, K. S. Kim, Dual Emission of Water-stable Two-Dimensional Organic-Inorganic Halide Perovskites with Mn(II) Dopant, Adv. Funct. Mater. 29, 1904768 (2019). (10.1002/adfm.201904768)
10. M. R. Rezapour, G. S. Lee, K. S. Kim, An effective approach to realize graphene based p-n junctions via adsorption of donor and acceptor molecules, Carbon 153, 525-530, 2019.
11. A. Jana, K. S. Kim, Effect of Organic-Cation Exchange Reaction of Perovskites in Water: H-bond Assisted Self-Assembly, Black Phase Stabilization, and Single-Particle Imaging, ACS Appl. Energy Mater. 1, 2, 4496-4503 (2019). doi.org/10.1021/acsaem.9b00742
12. A. Meena, M. Ha, S. S. Chandrasekaran, S. Sultan, P. Thangavel, A. M. Harzandi, B. Singh, J. N. Tiwari and K. S. Kim, Pt-like hydrogen evolution on V2O5/Ni(OH)2 electrocatalyst, J. Mater. Chem. A 7, 15794-15800 (2019). DOI: 10.1039/c9ta03627j
13. J. N. Tiwari, A. M. Harzandi, M. Ha, S. Sultan, C. W. Myung, H. J. Park, D. Y. Kim, P. Thangavel, A. N. Singh, P. Sharma, S. S. Chandrasekaran, F. Salehnia, J-W. Jang, H. S. Shin, Z. Lee, K. S. Kim, High-performance hydrogen evolution by Ru single-atoms and nitrided-Ru nanoparticles implanted on N-doped graphitic sheet, Adv. Ener. Mater. 9, 1900931 (2019). (cover).
14. D. Y. Kim, T. Yoon, Y. J. Jang, J. H. Lee, Y. Na, B. J. Lee, J. S. Lee, K. S. Kim, Band Gap Narrowing of Zinc Orthogermanate by Dimensional and Defect Modification, J. Phys. Chem. C 123, 14573-14581 (2019).

15. L. Wang, K. S. Kim, Signature of Quantum Dimensional Transition in Spin-1/2 Antiferromagnetic Heisenberg Model on A Square Lattice and Space Reduction in Matrix Product State, Phys. Rev. B 99, 134441 (2019).
16. S. Sultan, J. N. Tiwari, A. N. Singh, S. Zhumagali, M. Ha, C. W. Myung, P. Thangavel, K. S. Kim, Single Atoms and Clusters Based Nano-Materials for Hydrogen Evolution, Oxygen Evolution Reactions, and full Water Splitting, Adv. Ener. Mater. 9, 1900624 (2019). DOI: 10.1002/aenm.201900624
17. A. Jana, Q. Ba, K.S. Kim, Compositional and Dimensional Control of 2D and Quasi-2D Lead Halide Perovskites in Water, Adv. Funct. Mater. 29, 1900966 (2019). adfm.201900966
18. X. Li, J. Cui, Q. Ba, Z. Zhang, S. Chen, G. Yin, Y. Wang, B. Li, G. Xiang, K. S. Kim, H. Xu, Z. Zhang, and H.-L. Wang, Multiphotoluminescence from a Triphenylamine Derivative and Its Application in White Organic Light-Emitting Diodes Based on a Single Emissive Layer, Adv. Mater. 31, 1900613 (2019).
19. S.-H. Jeong, H. Kim, M.-H. Park, Y. Lee, N. Li, H.-K. Seo, T.-H. Han. S. Ahn, J.-M. Heo, K. S. Kim, T.-W. Lee, Ideal conducting polymer anode for perovskite light-emitting diodes by molecular interaction decoupling, Nano Energy 60, 324-331 (2019). DOI: 10.1016/j.nanoen.2019.03.030
20. A. Hajibabaei, K. S. Kim, First-order and continuous melting transitions in 2D Lennard-Jones systems and repulsive-disks, Phys. Rev. E 99, 022145 (2019).
21. G. Shi, M. A. Shahid, M. Yousuf, F. Mahmood, L. Rasheed, C. W. Bielawskiae, K. S. Kim, A ''turn-on'' fluorescent probe for the detection of permanganate in aqueous media, Chem. Commun. 55, 1470-1473 (2019). DOI: 10.1039/c8cc08958b
22. M. Filatov, S. K. Min, K. S. Kim, Non-Adiabatic Dynamics of Ring Opening in Cyclohexa-1,3-diene described by an Ensemble Density Functional Theory Method, Mol. Phys. 117, 1128-1141 (2019). DOI: 10.1080/00268976.2018.1519200
23. T. Yoon, G.-H. Kim, C. W. Myung, S. Kajal, J. Jeong, J. W. Kim, J. Y. Kim, and K. S. Kim, Ambient-Stable Cubic-Phase Hybrid Perovskite Reaching the Shockley–Queisser Fill Factor Limit via Inorganic Additive-Assisted Process, ACS Appl. Ener. Mater. 1, 5865-5871 (2018). DOI: 10.1021/acsaem.8b01364
24. C. W. Myung, G. Lee, K. S. Kim, La-doped BaSnO3 electron transport layer for perovskite solar cells, J. Mater Chem. A 6, 23071-23077 (2018). DOI: 10.1039/c8ta08764d
25. V. K. Singh, C. Yu, S. Badgujar, Y. Kim, Y. Kwon, D. Kim, J. Lee, T. Akhter, G. Thangavel, L. S. Park, J. Lee, P. C. Nandajan, R. Wannemacher, B. Milián-Medina, L. Lüer, K. S. Kim*, J. Gierschner*, M. S. Kwon* Highly efficient organic photocatalysts discovered via a computer-aided-design strategy for visible-light-driven atom transfer radical polymerization, Nature Catal. 1, 794-804 (2018).
26. S. Javaid, C. W. Myung, S. Pourasad, B. Rakshit, K. S. Kim,* and G. Lee*, Highly Hydrophobic Fluorographene based system as an Interlayer for Electron Transport in Organic-Inorganic Perovskite Solar Cells, J. Mater. Chem. A 6, 18635-18640 (2018).
27. A. Jana, K. S. Kim, Water-Stable, Fluorescent Organic−Inorganic Hybrid and Fully Inorganic Perovskites, ACS Energy Lett. 3, 2120-2126 (2018).
28. Michael Filatov, Marco Paolino, Seung Kyu Min, and Kwang S. Kim, Fulgides as Light-Driven Molecular Rotary Motors: Computational Design of a Prototype Compound, J. Phys. Chem. Lett. 9, 4995-5001 (2018). DOI: 10.1021/acs.jpclett.8b02268
29. J. N. Tiwari, S. Sultan, C. W. Myung, T. Yoon, N. Li, M. Ha, A. M. Harzandi, H. J. Park, D. Y. Kim, S. S. Chandrasekaran, W. G. Lee, V. Vij, H. Kang, T. J. Shin, H. S. Shin, G. Lee, Z. Lee, K. S. Kim, Multicomponent electrocatalyst with ultralow Pt loading and high hydrogen evolution activity, Nature Energy 3, 773-782 (2018). Doi: 10.1038/s41560-018-0209-x
30. T.-U. Yoon, S. B. Baek, D. Kim, E.-J. Kim, W.-G. Lee, B. Singh, M. S. Lah, Y.-S. Bae, K. S. Kim, Efficient Separation of C2 Hydrocarbons in a Permanently Porous Hydrogen-Bonded Organic Framework, Chem. Comm. 54, 9360-9363 (2018).
31. M. Filatov, S. K. Min, K. S. Kim, Direct Non-Adiabatic Dynamics by Mixed Quantum-Classical Formalism Connected with Ensemble Density Functional Theory Method: Application to trans-Penta-2,4-Dieniminium Cation, J. Chem. Theor. Comput. 14, 4499-4512 (2018), DOI: 10.1021/acs.jctc.8b00217
32. S. Sultan, J. N. Tiwari, J.-H. Jang, A. M. Harzandi, F. Salehnia, S. J. Yoo, K. S. Kim, Highly Efficient Oxygen Reduction Reaction Activity of Graphitic Tube Encapsulating Nitrided Co_xFe_y Alloy. Adv. Ener. Mater. 8, 1801002 (2018). DOI: 10.1002/aenm.201801002 (Back cover).
33. T. Yoon, G. Song, A. M. Harzandi, M. Ha, S. Choi, S. Shadman, J. Ryu, T. Bok, S. Park, and K. S. Kim, Intramolecular deformation of zeotype-borogermanate toward three-dimensional porous germanium anode for high-rate lithium storage, J. Mater. Chem. A 6, 15961-15967 (2018). (Back

Cover).

34. G. Shi, T. Yoon, S. Cha, S. Kim, M. Yousuf, N. Ahmed, D. Kim, H.-W. Kang, K. S. Kim, Turn-on and Turn-off Fluorescent Probes for Carbon Monoxide Detection and Blood Carboxyhemoglobin Determination. ACS Sensors, 3, 1102-1108 (2018). DOI: 10.1021/acssensors.8b00083
35. C. W. Myung, S. Javaid, K. S. Kim, G. Lee, Rashba-Dresselhaus Effect in Inorganic/Organic Lead Iodide Perovskite Interfaces, ACS Energy Lett. 3, 1294-1300 (2018).
36. S.-J. Kwon, T.-H. Han, T. Y. Ko, N. Li, Y. Kim, D. J. Kim, S.-H. Bae, Y. Yang, B. H. Hong, K. S. Kim, S. Ryu, and T.-W. Lee, Extremely stable graphene electrodes doped with macromolecular acid, **Nat. Commun.**9, 2037 (2018). DOI: 10.1038/s41467-018-04385-4
37. Y. Park, N. Li, G. Lee, K. S. Kim, K.-J. Kim, S. C. Hong, and S. W. Han, Sulfur-vacancy-dependent geometric and electronic structure of bismuth adsorbed on MoS_2, Phys. Rev. B 97, 115307 (2018).
38. C. W. Myung, J. Yun, G. Lee, K. S. Kim, A New Perspective on the Role of A-site Cations in Perovskite Solar Cells, Adv. Ener. Mater. 8, 1702898 (2018). DOI: 10.1002/aenm.201702898 (Back Cover).
39. S. Javaid, C. W. Myung, J. Yun, G. Lee, K. S. Kim, Organic Cation Steered Interfacial Electron Transfer within Organic-Inorganic Perovskite Solar Cell, J. Mater. Chem. A 6, 4305-4312 (2018) DOI: 10.1039/c7ta09504j. (Back Cover).
40. D. Y. Kim, D. C. M. Yang, J. M. L. Madridejos, A. Hajibabaei, C. Baig, K. S. Kim, Anisotropic and amphoteric charcteristics of diverse carbenes, Phys.Chem.Chem.Phys. 20,13722-13733(2018)..(Back Cover).
41. T. Yoon, J. Jun, D. Y. Kim, S. Pourasad, T. J. Shin, S. U. Yu, W. Na, J. Jang, K. S. Kim, An ultra-sensitive, flexible and transparent gas detection film based on well-ordered flat polypyrrole on single layered graphene, J. Mater. Chem. A 6, 2257-2263 (2018).
42. Seong Uk Yu, Hwiwon Lee, Woo Jong Cho, Chulhyun Kim, Moon Cheol Kang, Hyun-Joon Shin, Namdong Kim, Sei Kwang Hahn, Kwang S. Kim, Spectromicroscopic Observation of a Live Single Cell in a Biocompatible Liquid-Enclosing Graphene System, Nanoscale, 10, 150-157 (2018). DOI: 10.1039/C7NR05223E (Back Cover).
43. D. Kwon, J. Ryu, M. Shin, G. Song, D. Hong, K. S. Kim, S. Park, Synthesis of dual porous structured germanium anodes with exceptional lithium-ion storage performance, J. Power Sources, 274, 217-224 (2018).
44. D. K. L. Harijana, V. Chandra, T. Yoon, K. S. Kim, Radioactive iodine capture and storage from water using magnetite nanoparticles encapsulated in polypyrrole, J. Hazard. Mater. 344, 576-584 (2018).
45. Bhupendra Kumar Singh, Yongseon Kim, Seung Bin Baek, Abhishek Meenaa, Siraj Sultan, Ja HunKwak, Kwang S. Kim, Template Free Facile Synthesis of Mesoporous Mordenite for Bulky Molecular Catalytic Reactions, J. Indust. Eng. Chem. 57, 363-369 (2018).
46. Y.-K. Jeong, Y. M. Lee, J. Yun, T. Mazur, M. Kim, Y. J. Kim, M. Dygas, S. H. Choi, K. S. Kim, O.-H. Kwon, S. M. Yoon, B. A. Grzybowski, Tunable photoluminescence across the visible spectrum and photocatalytic activity of mixed-valence rhenium oxide nano-particles, J. Am. Chem. Soc. 139, 15088-15093 (2017) DOI: 10.1021/jacs.7b07494.
47. V. Vij, S. Sultan, A. M. Harzandi, A. Meena, J. N. Tiwari, W. -G. Lee, T. Yoon, K. S. Kim, Nickel–Based Electrocatalysts for Energy Related Applications: Oxygen Reduction, Oxygen Evolution, and Hydrogen Evolution Reactions, ACS Catal. 7, 7196-7225 (2017).
48. P. Dua, G. Lee, K. S. Kim, Ferromagnetism in Monatomic Chains: Spin-Dependent Bandwidth Narrowing/Broadening, J. Phys. Chem. C 121, 20994-21000 (2017).
49. J. N. Tiwari, W. G. Lee, S. Sultan, M. Yousuf, A. M. Harzandi, V. Vij, K. S. Kim, High-Affinity-Assisted Nanoscale Alloys as Remarkable Bifunctional Catalyst for Alcohol Oxidation and Oxygen Reduction Reactions, ACS Nano 11, 7729-7735 (2017). DOI: 10.1021/acsnano.7b01073
50. B. Park, K. Kim, J. Park, H. Lim, P. Lanh, A-R. Jang, C. Hyun, C. W. Myung, S. Park, J. W. Kim, K. S. Kim, H. S. Shin, G. Lee, S. Kim, J. K. Kim, C. Park, Anomalous Ambipolar Transport of Organic Semiconducting Crystals via Control of Molecular Packing Structures, ACS Appl. Mater. Interf. 9, 27839-27846 (2017).
51. M. R. Rezapour, C. W. Myung, J. Yun, A. Ghassami, N. Li, S. U. Yu, A. Hajibabaei, Y. Park, and K. S. Kim, Graphene and Graphene Analogs Towards Optical, Electronic, Spintronic, Green-Chemical, Energy-Material, Sensing, and Medical Applications, ACS Appl. Mater. Interf. 9, 24393-24406 (2017).
52. M. Filatov, T. J. Mart´ınez, K. S. Kim, Description of ground and excited electronic states by ensemble density functional method with extended active space, J. Chem. Phys. 147, 064104 (2017).
53. M. Ha, D. Y. Kim, N. Li, J. M. L. Madridejos, I. K. Park, I. S. Youn, J. Lee, C. Baig, M. Filatov, S. K. Min, G. Lee, K. S. Kim, Adsorption of Carbon Tetrahalides on Coronene and Graphene, J. Phys. Chem. C 121, 14968-14974 (2017). DOI: 10.1021/acs.jpcc.7b04939
54. T. Yoon, T. Bok, C. Kim, Y. Na, S. Park, K. S. Kim, Mesoporous Silicon Hollow Nanocubes Derived

from Metal Organic Framework Template for Advanced Lithium-Ion Battery Anode, ACS Nano 11, 4808-4815 (2017). 10.1021/acsnano.7b01185
55. Y. Park, S. W. Han, R. Taylor, C. C. Chan, B. Reid, Y. Jo, N. Kim, H. Im, K. S. Kim, Interplay between many body effects and Coulomb screening in optical bandgap of atomically thin MoS_2, Nanoscale 9, 10647 (2017). (back cover) doi.org/10.1039/c7nr01834g
56. D. Y. Kim, J. M. L. Madridejos, M. Ha, J.-H. Kim, D. C. Yang, C. Baig, K. S. Kim, Size-dependent conformational change in halogen–π interaction: from benzene to graphene, Chem. Comm. 53, 6140-6143 (2017). DOI: 10.1039/c7cc03116e
57. Y. Park, Y. Kim, C. W. Myung, R. A. Taylor, C. C. S. Chan, B. P. L. Reid, T. J. Puchtler, R. J. Nicholas, L. T. Singh, G. Lee, C.-C. Hwang, C.-Y. Park, and K. S. Kim, Two-Dimensional Excitonic Photoluminescence in Graphene on a Cu Surface, ACS Nano 11, 3207-3212 (2017). DOI: 10.1021/acsnano.7b00245 (http://arxiv.org/abs/1610.08630).
58. H. J. Lee, K. J. Korshavn, Y. Nam, J. Kang, T. J. Paul, R. A. Kerr, I. S. Youn, M. Ozbil, K. S. Kim, B. T. Ruotolo, R. Prabhakar, A. Ramamoorthy, M. H. Lim, Structural and Mechanistic Insights into Development of Chemical Tools to Control Individual and Inter-related Pathological Features in Alzheimer's Disease. Chem. Eur. J. 23, 2706-2715 (2017).
59. Tiwari, J. N.; Seo, Y.-K. ; Yoon, T.; Lee, W. G.; Cho, W. J.; Yousuf, M.; Harzandi, A. M. ; Kang, D.-S.; Kim, K.-Y.; Suh, P.-G.; Kim, K. S., Accelerated Bone-Regeneration by Two Photon Photoactivated Carbon Nitride Nanosheets, ACS Nano 11, 742-751 (2017).
60. A. M. Harzandi, J. N. Tiwari, H. S. Lee, H. C. Jeon, W. J. Cho, G. Lee, J. Baik, J.-H. Kwak, K. S. Kim, Efficient CO Oxidation by 50-Facet Cu2O Nanocrystals Coated with CuO Nanoparticles, ACS Appl. Mat. Interf., 9, 2495-2499 (2017).
61. Michael Filatov, Fang Liu, Kwang S. Kim, and Todd Martinez, Self-consistent implementation of ensemble density functional theory method for multiple strongly correlated electron pairs, J. Chem. Phys. 145, 244104 (2016).
62. M. R. Rezapour, J. Yun, G. Lee, K. S. Kim, Lower Electric Field-Driven Magnetic Phase Transition and Perfect Spin Filtering in Graphene Nanoribbons by Edge Functionalization, J. Phys. Chem. Lett. 7, 5049-5055 (2016). DOI: 10.1021/acs.jpclett.6b02437
63. H. Park, L. T. Singh, P. Lee, J. Kim, M. Rye, C.-C. Hwang, K. S. Kim, J. Chung, Observation of Mg-induced structural and electronic properties of graphene, Appl. Phys. Lett. 109, 193104 (2016).
64. I.-S. Youn, D. Y. Kim, W. J. Cho, J. M. L. Madridejos, H. M. Lee, M. Kolaski, J. Lee, C. Baig, S. K. Shin, M. Filatov, K. S. Kim, Halogen-π Interactions Between Benzene and X_2/CX_4 (X = Cl, Br): Assessment of Various Density Functionals with Respect to CCSD(T), J. Phys. Chem. A 120, 9305-9314 (2016).
65. T. Yoon, K. S. Kim, One step synthesis of CoS-doped β-Co(OH)2@amorphous MoS_2+x hybrid catalyst grown on nickel foam for high performance electrochemical overall water splitting, Adv. Funct. Mater. 41, 7386-7393 (2016).
66. M. Beck , J. Derrick , R. Kerr , S. B. Oh , W. J. Cho , S. J. Lee , Y. Ji , J. Han, Z. Tehrani, N. Suh, S. Kim, S. Larsen, K. S. Kim, J.-Y. Lee, B. Ruotolo, M. H. Lim, Structure-mechanism-based engineering of chemical regulators targeting distinct pathological factors in Alzheimer's disease, Nature Commun. 7, 13115 (2016). doi:10.1038/ncomms13115
67. H. Park, S. Choi, P. Lee, J. Kim, M. Ryu, K. S. Kim, J. Chung, Band and Bonding Characteristics of N_2^+ Ion-Doped Graphene. RSC Adv. 6, 84959-84964 (2016). DOI: 10.1039/C6RA19511C
68. S. K. Kim, W. Chen, S. Pourasad, and K. S. Kim, Two-Dimensional Icy Water Clusters Between a Pair of Graphene-Like Molecules or Graphene Sheets, J. Phys. Chem. C 120, 19212–19224 (2016).
69. V. Vij, J. N. Tiwari, and K. S. Kim, Covalent vs. Charge Transfer Modification of Graphene/Carbon-Nanotubes with Vitamin B1: Co/N/S-C Catalyst towards Excellent Oxygen Reduction. ACS Appl. Mater. Interf. 29, 16045-16052 (2016). DOI: 10.1021/acsami.6b03546
70. G. Shi, Z. A. Tehrani, D. Kim, W. J. Cho, I. S. Youn, H. M. Lee, M. Yousuf, N. Ahmed, B. Shirinfar, A. J. Teator, D. N. Lastovickova, L. Rasheed, M. S. Lah, C. W. Bielawski, K. S. Kim, Halides with Fifteen Aliphatic C–H···Anion Interaction Sites. Sci. Rep. 22, 30123 (2016).
71. L. Rasheed, M. Yousuf, I. S. Youn, G. Shi, K. S. Kim, An Efficient Non-Reaction Based Colorimetric and Fluorescent Probe for Highly Selective Discrimination of Pd^0 and Pd^{2+} in Aqueous Media. RSC Adv. 6, 60546-60549 (2016).
72. J. Yun, G. Lee, K. S. Kim, Electron Transport in Graphene Nanoribbon Field-Effect Transistor under Bias and Gate Voltages: Iso-Chemical Potential Approach. J. Phys. Chem. Lett. 7, 2478-2482 (2016). DOI: 10.1021/acs.jpclett.6b00996
73. T.-H. Han, S.-J. Kwon, N. Li, H.-K. Seo, W. Xu, K. S. Kim, T.-W. Lee, Versatile p-Type Chemical Doping to Achieve Ideal Flexible Graphene Electrodes, Angew. Chem. Int. Ed. 55, 6197-6201 (2016).

DOI: 10.1002/anie. 201600414R1
74. M. Yousuf, I. S. Youn, J. Yun, L. Rasheed, R. Valero, G. Shi, K. S. Kim, Violation of DNA Neighbor Exclusion Principle in RNA Recognition. Chem. Sci. 7, 3581-3588 (2016). DOI: 10.1039/C5SC03740A
75. M. Filatov, T. J. Martınez, K. S. Kim, Using the GVB Ansatz to develop ensemble DFT method for describing multiple strongly correlated electron pairs. Phys. Chem. Chem. Phys. 18, 21040-21060 (2016). DOI: 10.1039/C6CP00236F
76. A. D. DeAngelis, K. C. Kemp, N. Gaillard, K. S., Kim, Antimony(III) sulfide thin films as a photoanode material in photocatalytic water splitting, ACS Appl. Mat. Interf. 8, 8445-8451 (2016).
77. V. Georgakilas, J. Tiwari, K. C., Kemp, J. Perman, A. Bourlinos, K. S. Kim, R. Zboril, Non-Covalent Functionalization of Graphene and Graphene Oxide for Energy Materials, Biosensing, Catalytic, and Biomedical Applications, **Chem. Rev.** 116, 5464-5519 (2016).
78. S. Y. Willow, X. C. Zeng, S. S. Xantheas, K. S. Kim, S. Hirata, Why Is MP2-Water "Cooler" and "Denser" than DFT-Water? J. Phys. Chem. Lett. 7, 680-684 (2016).
79. V. Vij, J. N Tiwari, W.-G. Lee, T. Yoon, K. S. Kim, Hemoglobin-carbon nanotube derived noble-metal-free Fe5C2-based catalyst for highly efficient oxygen reduction reaction, Sci. Rep 6, 20132 (2016). doi: 10.1038/srep20132.
80. Z. A. Tehrani, K. S. Kim, Functional Molecules and Materials by π-interaction Based Quantum Theoretical Design, Int. J. Quant. Chem. 116, 622-633 (2016).
81. I. S. Youn, W. J. Cho, K. S. Kim, Effects of an Electric Field on Interaction of Aromatic Systems. J. Comput. Chem. 37, 971-975 (2016).
82. J. N. Tiwari, V. Vij, K. C. Kemp, K. S. Kim, Engineered Carbon-Nanomaterial Based Electrochemical Sensors for Biomolecules, ACS Nano 10, 46-80 (2016). DOI: 10.1021/acsnano.5b05690
83. K. L. V. Joseph, A. Anthonysamy, R. Easwaramoorthi, D. V. Shinde, V. Ganapathy, S. Karthikeyan, J. Lee, T. Park, S.-W. Rhee, K. S. Kim, J. K. Kim, Cyanoacetic acid tethered thiophene for well-matched LUMO level in Ru(II)-terpyridine dye sensitized solar cells, Dyes and Pigments 126, 270-278 (2016) DOI: 10.1016/j.dyepig.2015.12.007
84. S. W. Han, W. S. Yun, J. D. Lee, Y. H. Hwang, J. Baik, H. J. Shin, W. G. Lee, Y. S. Park, and K. S. Kim, Hydrogenation-induced atomic stripes on the 2H−MoS_2 surface. Phys. Rev. B 92, 241303(R) (2015).
85. P. Lee, K.-H. Jin, S. J. Sung, J. G. Kim, M.-T. Ryu, H.-M. Park, S.-H. Jhi, N. Kim, Y. Kim, S. U. Yu, K. S. Kim, D. Y. Noh, J. Chung, Proximity Effect Induced Electronic Properties of Epitaxial Graphene on Bi2Te2Se, ACS Nano 9, 10861-10866 (2015).
86. M. Shabbaghi, H. W. Lee, T. Stauber, K. S. Kim, Drift-induced modifications to the dynamical polarization of graphene, Phys. Rev. B 92, 195429 (2015).
87. S. B. Baek, D. Moon, R. Graf, W. J. Cho, S. W. Park, T.-U. Yoon, S. J. Cho, I.-C. Hwang, Y.-S. Bae, H. W. Spiess, H. C. Lee, K. S. Kim, High-Temperature in situ Crystallographic Observation of Reversible Gas Sorption in Impermeable Organic Cages, Proc. Nat. Acad. Sci. 112, 14156-14161 (2015).
88. S. K. Kim, H. M. Lee, K. S. Kim, Disulfuric acid dissociated by two water molecules: Ab initio and density functional theory calculations, Phys. Chem. Chem. Phys. 17, 28556-28564 (2015). (back cover)
89. H. Kim, V. D. Doan, W. J. Cho, R. Valero, Z. A. Tehrani, J. M. L. Madridejos, K. S. Kim, Intriguing Electrostatic Potential of CO: Negative Bond-ends and Positive Bond-cylindrical-surface. Sci. Rep. 5, 16307 (2015).
90. L. Rasheed, M. Yousuf, I. S. Youn, T. Yoon, K.-Y. Kim, Y.-K. Seo, G. Shi, J.-H. Hur, K. S. Kim, Turn-on Ratiometric Fluorescent Probe for Selective Discrimination of Cr3+ from Fe3+ in Aqueous Media for Living Cell Imaging, Chem. Eur. J. 21, 16349-16353 (2015).
91. S. Y. Willow, M. A. Salim, .K. S. Kim, S. Hirata, Ab initio molecular dynamics of liquid water using embedded fragment second-order many-body perturbation theory towards its accurate property prediction. Sci. Rep. 5, 14358 (2015).
92. C. K. Kemp, S. B. Baek, W. G. Lee, M. Meyyappan, K. S. Kim, Activated carbon derived from waste coffee grounds for stable methane storage. Nanotech. 26, 385602 (2015).
93. B. Park, J. Park, J. G. Son, Y.-J. Kim, S.-U. Yu, H. J. Park, D.-H. Chae, J. Byun, G. Jeon, S. Huh, S.-K. Lee, A. Mishchenko, S. Hyun, T. G. Lee, S. W. Han, J.-H. Ahn, Z. Lee, C. Hwang, K. S. Novoselov, K. S. Kim, B. H. Hong, J. K. Kim, A Facile Route for Patterned Growth of Metal-Insulator Carbon Lateral Junction through One-pot Synthesis, ACS Nano, 9, 8352-8360 (2015). DOI 10.1021/acsnano.5b03037
94. Y. S. Park, G. Lee, M. Holmes, C. C. S. Chan, B. Reid, J. A. Alexander-Webber, R. J. Nicolas, R. Taylor, K. S. Kim, S. W. Han, W. Yang, Y. Jo, J. Kim, H. Im, Surface Effect Induced Optical Bandgap

Shrinkage in GaN Nanotubes, Nano Lett., 15, 4472-4476 (2015). DOI: 10.1021/acs.nanolett.5b00924
95. H. M. Lee, K. H. Lee, G. Lee, and K. S. Kim, Geometrical and Electronic Characteristics of $AunO_2^-$ (n=2-7), J. Phys. Chem. C 119, 14383-14391 (2015). DOI 10.1021/acs.jpcc.5b03051
96. C. Hyun, J. Yun, W. J. Cho, C. W. Myung, J. Park, G. Lee, Z. Lee, K. Kim, and K. S. Kim, Graphene Edges and Beyond: Temperature Driven Structures and Electromagnetic Properties. ACS Nano 9, 4669-4674 (2015). DOI: 10.1021/acsnano.5b02617
97. M. Saleh and K. S. Kim, Highly selective CO2 adsorption performance of carbazole based microporous polymers, RSC Adv. 5, 41745-41750 (2015).
98. H. H. Kim, B. Kang, J. W. Suk, N. Li, K. S. Kim, R. S. Ruoff, W. H. Lee, K. Cho, Clean Transfer of Wafer-Scale Graphene via Liquid Phase Removal of Polycyclic Aromatic Hydrocarbons, ACS Nano 9, 4726-4733 (2015).
99. H. M. Lee, I. S. Youn, M. Saleh, J. W. Lee, K. S. Kim, Interactions of CO_2 with various functional molecules, Phys. Chem. Chem. Phys. 17, 10925-10933 (2015). DOI: 10.1039/C5CP00673b
100. N. Li, G. Lee, Y. H. Jeong, K. S. Kim, Tailoring Electronic and Magnetic Properties of MoS_2 Nanotubes, J. Phys. Chem. C 119, 6405-6413 (2015). DOI: 10.1021/acs.jpcc.5b00176
101. M. Saleh, S. B. Baek, H. M. Lee, K. S. Kim, Triazine-Based Microporous Polymers for Selective Adsorption of CO_2, J. Phys. Chem. C. 119, 5395-5402 (2015). DOI: 10.1021/jp509188h
102. M. Kocman, P. Jurecka, M. Dubecky, M. Otyepka, Y. Cho, and K. S. Kim, Choosing a Density Functional for Modeling Adsorptive Hydrogen Storage: Reference Quantum Mechanical Calculations and a Comparison of Dispersion-Corrected Density Functionals, Phys. Chem. Chem. Phys. 17, 6423-6432 (2015).
103. W. Xu, L. Wang, Y. Liu, S. Thomas, H.-K. Seo, K.-I. Kim, K. S. Kim, T.-W. Lee, Controllable n-type doping on CVD-grown single- and double-layer graphene mixture, Adv. Mater. 27, 1619-1623 (2015). DOI: 10.1002/adma.201405353
104. S. K. Min, A. Abedit, K. S. Kim, E. K. U. Gross, Is the molecular Berry phase an artifact of the Born-Oppenheimer approximation? Phys. Rev. Lett. 113, 263004 (2014).
105. Y. Cho, W. J. Cho, I. S. Youn, G. Lee, N. J. Singh, and K. S. Kim, Density Functional Theory Based Study of Molecular Interactions, Recognition, Engineering, and Quantum Transport in π Molecular Systems, Acc. Chem. Res. 47, 3321-3330 (2014).
106. S. Y. Willow, K. S. Kim, and S. Hirata, Brueckner-Goldstone quantum Monte Carlo for correlation energies and quasiparticle energy bands of one-dimensional solids, Phys. Rev. B 90, 201110(R) (2014).
107. S. Thomas and K. S. Kim, Linear and Nonlinear Optical Properties of Indeno[2,1-b]fluorene and its Structural Isomers, Phys. Chem. Chem. Phys. 16, 24592-24597 (2014).
108. S. U. Yu, B. Park, Y. Cho, S. Hyun, J. K. Kim, K. S. Kim, Simultaneous Visualization of Graphene Grain Boundaries and Wrinkles with Structural Information by Gold Deposition, ACS Nano 8. 8662-8668 (2014). DOI: 10.1021/nn503550d
109. M. R. Rezapour, A. C. Rajan, and K. S. Kim, Molecular sensing using armchair graphene nanoribbon, J. Comput. Chem. 35, 1916-1920 (2014).
110. Y. S. Park, J. H. Park, H. N. Hwang, T. S. Laishram, K. S. Kim, M. H. Kang, and C. C. Hwang, Quasi-Free-Standing Graphene Monolayer on a Ni Crystal through Spontaneous Na Intercalation, Phys. Rev. X 4, 031016 (2014).
111. S. K. Lee, J. W. Yang, H. H. Kim, S. B. Jo, B. Kang, H. Bong, H. C. Lee, G. Lee, K. S. Kim, and K. Cho, Inverse Transfer Method Using Polymers with Various Functional Groups for Controllable Graphene Doping, ACS Nano 8, 7968-7975 (2014). DOI: 10.1021/nn503329s
112. J. Tucek, K. C. Kemp, K. S. Kim, and R. Zboril, Iron Oxide Supported Nanocarbon in Lithium-Ion Batteries, Medical, Catalytic, and Environmental Applications, ACS Nano 8, 7571-7612 (2014).
113. H. Kim, V. D. Doan, W. J. Cho, M. V. Madhav, and K. S. Kim, Anisotropic Charge Distribution and Anisotropic van der Waals Radius Leading to Intriguing Anisotropic Noncovalent Interactions, Sci. Rep. 4, 5826 (2014).
114. W. J. Cho, J. Kim, J. Lee, T. Keyes, J. E. Straub, K. S. Kim, Limit of metastability for liquid and vapor phases of water, Phys. Rev. Lett. 112, 157802 (2014). DOI: 10.1103/PhysRevLett.112.157802
115. M. Yousuf, N. Ahmed, B. Shirinfar, V. M. Miriyala, I. S. Youn, K. S. Kim, Precise Tuning of Cationic Cyclophanes toward Highly Selective Fluorogenic Recognition of Specific Biophosphate Anions, Org. Lett. 16, 2150-2153 (2014). DOI: 10.1021/ol500613y
116. S. Thomas, A. C. Rajan, M. R. Rezapour, K. S. Kim, In Search of a Two Dimensional Material for DNA Sequencing, J. Phys. Chem. C 118, 10855-10858 (2014).
117. M. Saleh, H. M. Lee, M., K. C. Kemp, K. S. Kim, Highly stable CO_2/N_2 and CO_2/CH_4 selectivity in hypercrosslinked heterocyclic porous polymers, ACS Appl. Mater. Interf. 6, 7325-7333 (2014).

118. H. M. Lee, I. S. Youn, K. S. Kim, CO Capture and Conversion to HOCO Radical by Ionized Water Clusters, J. Phys. Chem. A 118, 7274-7279 (2014) DOI: 10.1021/jp410927a
119. D. Kim, X. Liu, M. Oh, X. Song, Y. Zou, D. Singh, K. S. Kim, and M. S. Lah, Isoreticular metal-organic frameworks based on a rhombic dodecahedral metal-organic polyhedron as a tertiary building unit, CrystEngComm. 16, 6391-6397 (2014). DOI: 10.1039/C4CE00017J
120. A. C. Rajan, M. R. Rezapour, J. Yun, Y. Cho, W. J. Cho, S. K. Min, G. Lee, and K. S. Kim, Two Dimensional Molecular Electronics Spectroscopy for Molecular Fingerprinting, DNA Sequencing and Cancerous DNA Recognition, ACS Nano 8, 1827-1833 (2014). DOI: 10.1021/nn4062148
121. N. Kim, P. Lee, Y. Kim, J. S. Kim, Y. Kim, D. Y. Noh, S. U. Yu, J. Chung, and K. S. Kim, Persistent Topological Surface State at the Interface of Bi_2Se_3 Film Grown on Patterned Graphene, ACS Nano 8, 1154-1160 (2014). DOI: 10.1021/nn405503k
122. S. J. Sung, J. W. Yang, P. R. Lee, J. G. Kim, M. T. Ryu, H. M. Park, G. Lee, C. C. Hwang, K. S. Kim, J. S. Kim, J. W. Chung, Spin-induced band modifications of graphene through intercalation of magnetic iron atoms, Nanoscale 6, 3824 (2014). DOI: 10.1039/C3NR04178F
123. G. Shi, C. G. Gadhe, S. W. Park, K. S. Kim, J. Kang, H. Seema, N. J. Singh, S. J. Cho, Novel Ionophores with 2n-Crown-n Topology: Anion Sensing via Pure Aliphatic C-H center dot center dot center dot Anion Hydrogen Bonding, Org. Lett. 16, 334-337 (2014). DOI: 10.1021/ol402819m
124. H. Seema, K. C. Kemp, N. H. Le, S.-W. Park, V. Chandra, J. W. Lee, K. S. Kim, Highly selective CO_2 capture by S-doped microporous carbon materials, Carbon 66, 320-326 (2014).
125. Y. J. Hong, J. W. Yang, W. H. Lee, R. Ruoff, K. S. Kim, T. Fukui, Van der Waals Epitaxial Double Heterostructure: InAs/Single-Layer Graphene/InAs, Adv. Mater. 25, 6847-6853 (2013). (back cover). DOI: 10.1002/adma.201302312
126. J. Jang, J. Park, S. Nam, J. E. Anthony, Y. Kim, K. S. Kim, K. S. Kim, B. H. Hong, C. Park, Self-organizing properties of triethylsilylethynyl-anthradithiophene on monolayer graphene electrodes in solution-processed transistors, Nanoscale 5, 11094-11101 (2013). DOI: 10.1039/c3nr03356b
127. Tiwari, Jitendra N.; Kemp, K. Christian; Nath, Krishna; Tiwari, Rajanish; Nam, Hong Gil; Kim, Kwang, Interconnected Pt-Nanodendrite/DNA/Reduced-Graphene-Oxide Hybrid Showing Remarkable Oxygen Reduction Activity and Stability, ACS Nano 7, 9223-9231 (2013). DOI: 10.1021/nn4038404.
128. S. Yoo Willow, M. R. Mattew, K. S. Kim, S. Hirata, Convergence acceleration of parallel Monte Carlo second-order many-body perturbation calculations using redundant walkers, J. Chem. Theor. Comput. 9, 43296-4402 (2013). DOI: 10.1021/ct400557z.
129. T. Kim, J. Park, H. J. Jin, H. Lee, K.-E. Byun, C.-S. Lee, K. S. Kim, B. H. Hong, T. H. Kim, S. Hong, Graphene nanonet for biological sensing applications, Nanotech. 24, 375302 (2014). doi:10.1088/0957-4484/24/37/375302
130. N. H. Le., H. Seema, K. C. kemp, N. Ahmed, J. N. Tiwari, S. Park, K. S. Kim, Solution-Processable Micro-Hydrogels of Nanoparticle/Graphene Platelets Produced by Reversible Self-Assembly and Aqueous Exfoliation, J. Mater. Chem. A 2013, 1, 12900-12908. DOI: 10.1039/C3TA12735D
131. N. Ahmed, B. Shirinfar, I. S. Youn, M. Yousuf, K. S. Kim, Selective Detection of Guanosine-5′-triphosphate and Iodide by Fluorescent Benzimidazolium-based Cyclophanes, Org. Biomol. Chem. (11, 6407-6413 (2013). DOI: 10.1039/C3OB41470A
132. J. N. Tiwari, K. Nath, S. Kumar, R. N. Tiwari, K.C. Kemp, N. H. Le, D. H. Youn, J. S. Lee, K. S. Kim, Stable Pt nanoclusters on genomic DNA-graphene oxide with a high oxygen reduction reaction activity, **Nature Commun.** 4, 2221 (2013). DOI: 10.1038/ncomms32221
133. J. N. Tiwari, R. N. Tiwari, G. Singh, K. S. Kim, Recent progress in the development of anode and cathode catalysts for direct methanol fuel cells, Nano Energy 2013, 2, 553-578, http://dx.doi.org/10.1016/j.nanoen. 2013.06.009
134. C. Jeon, H.-N. Hwang, W.-G. Lee, Y. G. Jung, K. S. Kim, C.-Y. Park, C.-C. Hwang, Rotated domains in chemical vapor deposition-grown monolayer graphene on Cu(111): an angle-resolved photoemission study, Nanoscale 5, 8210- 8214 (2013). DOI: 10.1039/C3NR01700A
135. J. Y. Lee, B. H. Hong, D. Y. Kim, D. R. Mason, J. W. Lee, Y. Chun, and Kwang S. Kim, Tuning Molecular Self-Assembly Toward Intriguing Nanomaterial Architectures, Chem. Eur. J. 19, 9118-9122 (2013). DOI: 10.1002/chem.201204263
136. Y. Chun, N. J. Singh, I.-C. Hwang, J. W. Lee, S. U. Yu, and K. S. Kim, Calix[n]imidazolium as a new class of positively charged homocalix compounds, **Nature Commun.** 4, 1797 (2013). DOI: 10.1038/ncomms2758
137. S. W. Han, Y. Hwang, S.-H. Kim, W. S. Yun, J. D. Lee, M. G. Park, S. Ryu, J. S. Park, D.-H. Yoo, S.-P. Yoon, S. C. Hong, K. S. Kim, Y. S. Park, Controlling ferromagnetic easy axis in a layered MoS_2 single crystal, Phys. Rev. Lett. 110, 247201 (2013).
138. H. M. Lee, K. S. Kim, Dynamics and Structural Changes of Small Water Clusters upon Ionization, J. Comput. Chem. 34, 1589-1597 (2013). DOI: 10.1002/jcc.23296

139. M. Saleh, K. C. Kemp, N. H. Le, K. S. Kim, Synthesis of N-doped microporous carbon via chemical activation of polyindole-modified graphene oxide sheets for selective carbon dioxide adsorption, Nanotech. 24, 255702 (2013).
140. S. U. Yu, Y. Cho, B. Park, N. Kim, I. S. Youn, M. Son, J. K. Kim, H. C. Choi, K. S. Kim, Fast benchtop visualization of graphene grain boundaries using adhesive properties of defects, Chem. Commun. 49, 5474-5476 (2013).
141. M. Saleh, J. N. Tiwari, K. C. Kemp, M. Yousuf, K. S. Kim, Highly selective and stable carbon dioxide uptake in polyindole-derived microporous carbon materials, Env. Sci. Tech. 47, 5467-5473 (2013). DOI: 10.1021/es3052922
142. K. C. Kemp, V. Chandra, M. Saleh, K. S. Kim, Reversible CO_2 adsorption by an activated nitrogen doped graphene/polyaniline material, Nanotech. 24, 235703 (2013).
143. S. Y. Willow, K. S. Kim, and S. Hirata, Stochastic evaluation of second-order Dyson self-energies, J. Chem. Phys. 138, 164111 (2013). doi: 10.1063/1.4801862.
144. Y. Cho, S. K. Min, J. Yun, W. Y. Kim, A. Tkatchenko, and K. S. Kim, Noncovalent Interactions of DNA Bases with Naphthalene and Graphene, J. Chem. Theory Comput. 9, 2090-2096 (2013). DOI: 10.1021/ct301097u
145. K. C. Kemp, H. Seema, M. Saleh, N. H. Le, K. Mahesh, V. Chandra, and K. S. Kim, Environmental applications using graphene composites: water remediation and gas adsorption, Nanoscale 5, 3149-3171 (2013). DOI: 10.1039/C3NR33708A
146. H. H. Kim, J. W. Yang, S. B. Jo, B. Kang, S. K. Lee, H. Bong, G. Lee, K. S. Kim, and K. Cho, Substrate-Induced Solvent Intercalation for Stable Graphene Doping, ACS Nano 7, 1155-1162 (2013).
147. N. Li, G. Lee, J. W. Yang, H. Kim, M. S. Yeom, R. Scheicher, J. S. Kim, and K. S. Kim, Non-Covalent Functionalization with Alkali Metal to Separate Semiconducting from Metallic Carbon Nanotubes: A Theoretical Study, J. Phys. Chem. C 117, 4309-4313 (2013).
148. J. N. Tiwari, K. Mahesh, N. H. Le, K. C. Kemp, R. Timilsina, R. N. Tiwari, and K. S. Kim, Reduced graphene oxide-based hydrogels for the efficient capture of dye pollutants from aqueous solutions, Carbon 56, 173-182 (2013).
149. B. Shirinfar, N. Ahmed, Y. S. Park, G.-S. Cho, I. S. Youn, J.-K. Han, H. G. Nam, and K. S. Kim, Selective fluorescent detection of RNA in living cells by using imidazolium-based cyclophane, J. Am. Chem. Soc. 135, 90-93 (2013).
150. S. K. Seth, P. Manna, N. J. Singh, M. Mitra, A. D. Jana, A. Das, S. R. Choudhury, T. Kar, S. Mukhopadhyay, and K. S. Kim, Molecular architecture using novel types of non-covalent π-interactions involving aromatic neutrals, aromatic cations and π-anions, CrystEngComm. 15, 1285-1288 (2013).
151. M. Kolaski, C. R. Arunkumar, K. S. Kim, Aromatic excimers: ab initio and TD-DFT study, J. Chem. Theory Comput. 9, 847-856 (2013).
152. S. Choi, J. Chung, and K. S. Kim, Relation between primes and nontrivial zeros in the Riemann hypothesis; Legendre polynomials, modified zeta function and Schrodinger equation, J. Math. Phys. 53, 122108 (2012). DOI: **10.1063/1.4770050**
153. S. Y. Willow, K. S. Kim, S. Hirata, Stochastic evaluation of second-order many-body perturbation energies, J. Chem. Phys. 137, 204122 (2012).
154. V. Georgakilas, M. Otyepka, A. B. Bourlinos, V. Chandra, N. Kim, K. C. Kemp, P. Hobza, R. Zboril, and K. S. Kim, Functionalization of Graphene: Covalent and noncovalent approaches, derivatives and applications, **Chem. Rev.** 112, 6156-6214 (2012).
155. S. D. Kunikeev and K. S. Kim, Cumulant expansion and analytic continuation in Monte Carlo simulation of classical Lennard-Jones clusters, Phys. Rev. E. 86, 056702 (2012).
156. A. Tkatchenko, D. Alfe, and K. S. Kim, First-Principles Modeling of Non-Covalent Interactions in Supramolecular Systems: The Role of Many-Body Effects, J. Chem. Theory Comput. 8, 4317-4322. (2012).
157. G. Lee, H. S. Ji, Y. Kim, C. Kim, K. Haule, G. Kotliar, B. Lee, S. Khim, K. H. Kim, K. S. Kim, K.-S. Kim, J. H. Shim, Orbital selective Fermi surface shifts and mechanism of high Tc superconductivity in correlated AFeAs (A=Li,Na), Phys. Rev. Lett. 109, 177001 (2012).
158. S. Myung, C. Kim, P. T. Yin, J. Park, A. Solanki, P. I. Reyes, Y. Lu, K. S. Kim, and K.-B. Lee, Label-free polypeptide-based enzyme detection using a graphene-nanoparticle hybrid sensor, Adv. Mater. 24, 6081-6087 (2012).
159. H. M. Lee and K. S. Kim, Observable Structures of Small Neutral and Anionic Gold Clusters, Chem. Eur. J. 18,13203-13207 (2012).
160. Y. S Park, M. J. Holmes, R. A. Taylor, K. S. Kim, S.-W. Lee, H. Ju, and H. Im, Selective self-

assembly and characterization of GaN nanopyramids on m-plane InGaN/GaN quantum disks, Nanotech. 23, 405602 (2012).

161. H. Seema, C. C. Kemp, V. Chandra, K. S. Kim, Graphene-SnO_2 composites for highly efficient photocatalytic degradation of methylene blue under sunlight, Nanotech. 23, 355705 (2012).
162. S.-W. Park, Y. Chun, S. J. Cho, S. Lee, K. S. Kim, Design of Carbene-based Organocatalysts for Nitrogen Fixation: Theoretical Study, J. Chem. Theory Comput. 8, 1983-1988 (2012).
163. D. R. Mason, D. K. Gramotnev, and K. S. Kim, Plasmon nanofocusing in a dielectric hemisphere covered in tapered metal film, Opt. Exp. 20, 12866-12876 (2012).
164. W. H. Lee, J. W. Suk, H. Chou, J. Lee, Y. Hao, Y. Wu, R. Piner, D. Akinwande, K. S. Kim, and R. S. Ruoff, Selective-Area Fluorination of Graphene with Fluoropolymer and Laser Irradiation, Nano Lett. 12, 2374-2378 (2012).
165. E. Jung, K. S. Kim, and D. Park, Time dependence of the position momentum and position velocity uncertainties in gapped graphene, Phys. Rev. B 85, 165418 (2012).
166. H. Lee, K. Heo, J. Park, Y. Park, S. Noh, K. S. Kim, C. Lee, B. H. Hong, J. Jian, and S. Hong, Graphene-Nanowire Hybrid Structures for High-performance Photoconductive Devices, J. Mater. Chem. 22, 8372-8376 (2012).
167. W. H. Lee, J. W. Suk, J. Lee, Y. Hao, J. Park, J. W. Yang, H.-W. Ha, S. Murali, H. Chou, D. Akinwande, K. S. Kim, and R. S. Ruoff, Simultaneous Transfer and Doping of CVD-grown Graphene by Fluoropolymer for Transparent Conductive Films on Plastic, ACS Nano 6, 1284-1290 (2012).
168. V. Suresh, N. Ahmed, I. S. Youn, K. S. Kim, An Imidazolium-Based Fluorescent Cyclophane for the Selective Recognition of Iodide, Chem. Asian J. 7, 658-663 (2012).
169. J. N. Tiwari, R. N. Tiwari, and K. S. Kim, Zero–dimensional, one–dimensional, two–dimensional and three–dimensional nanostructured materials for advanced electrochemical energy devices, Prog. Mater. Sci. 57, 724-803 (2012).
170. M. Jouravlev, D. R. Mason, and K. S. Kim, Ultralow Raman lasing threshold and enhanced gain of whispering gallery modes in silica microspheres, Phys. Rev. A 85, 013825 (2012).
171. J. Park, S. B. Jo, Y.-J. Yu, Y. Kim, J. W. Yang, W. H. Lee, H. H. Kim, B. H. Hong, P. Kim, K. Cho, and K. S. Kim, Single-gate bandgap opening of bilayer graphene by dual molecular doping, Adv. Mater. 24, 407-411 (2012).
172. N. Ahmed, V. Suresh, B. Shirinfar, I. Geronimo, A. Bist, I.-C. Hwang, and K. S. Kim, Fluorogenic Sensing of $CH_3CO_2^-$ and $H_2PO_4^-$ by Ditopic Receptor through Conformational Change, Org. Biomol. Chem. 10, 2094-2100 (2012).
173. N. Ahmed, B. Shirinfar, I. S. Youn,A. Bist, V. Suresh, K. S. Kim, A highly selective fluorescent chemosensor for guanosine-5'-triphosphate via excimer formation in aqueous solution of physiological pH, Chem. Commun. 48, 2662-2664 (2012). [inside front cover]
174. D. Y. Kim, I. Geronimo, N. J. Singh, H. M. Lee, K. S. Kim, Anion Binding by Electron-Deficient Arenes Based on Complementary Geometry and Charge Distribution, J. Chem. Theory Comput. 8, 274-280 (2012).
175. I. S. Youn, D. Y. Kim, N. J. Singh, S. W. Park, J. Youn, K. S. Kim, Intercalation of transition metals into stacked benzene rings: A model study of the intercalation of transition metals into bi-layered graphene, J. Chem. Theory Comput. 8, 99-105 (2012).
176. V. Chandra, S. U. Yu, S. Kim, Y. S. Yoon, D. Y. Kim, A. H. Kwon, M. Meyyappan, and K. S. Kim, Highly Selective CO_2 Capturing on N-doped Carbon Produced by Chemical Activation of Polypyrrole Functionalized Graphene Sheets, Chem. Commun. 48, 735-737 (2012).
177. S. K. Min, Y. Cho, K. S. Kim, Efficient electron dynamics with the planewave-based real-time time-dependent density functional theory: absorption spectra, vibronic electronic spectra, and coupled electron-nucleus dynamics, J. Chem. Phys. 135, 244112 (2011).
178. S. Huh, J. Park, Y. S. Kim, K. S. Kim, B. H. Hong, and J. M. Nam, UV/Ozone-Oxidized Large-Scale Graphene Platform with Large Chemical Enhancement in Surface-Enhanced Raman Scattering, ACS Nano 5, 9799-9806 (2011).
179. H. M. Lee and K. S. Kim, Water trimer cation: Theor. Chem. Acc. 130, 543-548 (2011).

180. Y.-J. Yu, M. Y. Han, S. Berciaud, A. B. Georgescu, T. F. Heinz, L. E. Brus, K. S. Kim, and P. Kim, High-resolution spatial mapping of the temperature distribution of a Joule self-heated graphene nanoribbon, Appl. Phys. Lett. 99, 183105 (2011).
181. K. S. Kim, S. Karthikeyan, and N. J. Singh, How different are aromatic π interactions from aliphatic π interactions and non-π stacking interactions?, J. Chem. Theory Comput. 7, 3471-3477 (2011).
182. S. Y. Willow, N. J. Singh, K. S. Kim, NH4+ Resides Inside the Water 20-mer Cage As Opposed to H_3O+, Which Resides on the Surface: A First Principles Molecular Dynamics Simulation Study, J. Chem. Theory Comput. 7, 3461-3465 (2011).
183. J. W. Yang, G. Lee, J. S. Kim, and K. S. Kim, Gap Opening of Graphene by Dual $FeCl_3$ Acceptor and K Donor Doping, J. Phys. Chem. Lett. 2, 2577-2581 (2011).
184. N. Ahmed, B. Shirinfar, I. Geronimo, and K. S. Kim, Fluorescent Imidazolium-based Cyclophane for Detection of Guanosine-5'-triphosphate and I^- in Aqueous Solution of Physiological pH, Org. Lett. 13, 5476-5479 (2011).
185. S. W. Park, C. W. Kim, J. H. Lee, G. Shim, and K. S. Kim, Comparison of arsenic acid with phosphoric acid in the interaction with a water molecule and an alkali/alkaline-earth metal cation, J. Phys. Chem. A 115, 11355-11361 (2011).
186. M. Kolaski, A. Zakharenko, S. Karthikeyan, and K. S. Kim, Structures, energetics, and IR spectra of monohydrated inorganic acids: Ab initio and DFT study, J. Chem. Theor. Comput. 7, 3447-3459 (2011).
187. S. Y. Park, J. Park, S. H. Sim, M. G. Sung, K. S. Kim, B. H. Hong, and S. H. Hong, Enhanced Differentiation of Human Neural Stem Cells into Neurons on Graphene, Adv. Mater. 23, H263-267, (2011).
188. J. W. Yi, J. Park, K. S. Kim, B. H. Kim, pH-Responsive Self-Duplex of PyA-Substituted Oligodeoxyadenylate in Graphene Oxide Solution as a Molecular Switch, Org. Biomol. Chem. 9, 7434-7438 (2011).
189. S. Y. Shin, N. D. Kim, J. G. Kim, K. S. Kim, D. Y. Noh, K. S. Kim, and J. W. Chung, Control of the π plasmon in a single layer graphene by charge doping, Appl. Phys. Lett. 99, 082110 (2011).
190. H. Jabeen, V. Chandra, S. Jung, J. W. Lee, K. S. Kim, and S. B. Kim, Enhanced Cr(VI) removal using iron nanoparticle decorated graphene, Nanoscale 3, 3583-3585 (2011).
191. J. Wang, K. S. Kim, and E. J. Baerends, Electron pair density in the lowest $^1\Sigma^{u+}$ and $^1\Sigma^{g+}$ states of H_2, J. Chem. Phys. 135, 074111 (2011).
192. S. K. Min, Y. Cho, D. R. Mason, J. Lee, and K. S. Kim, Theoretical Design of Nanomaterials and Nanodevices – Nanolensing, Supermagnetoresistance, and Ultrafast DNA Sequencing, J. Phys. Chem. C (feature article) 115, 16247-16257 (2011). (cover).
193. A. Anthonysamy, Y. Lee, B. Karunagaran, V. Ganapathy, S.-W. Rhee, S. Karthikeyan, K. S. Kim, M. J. Ko, N.-G. Park, M.-J. Ju, and J. K. Kim, Molecular design and synthesis of ruthenium(II) sensitizers for highly efficient dye-sensitized solar cells, J. Mater. Chem. 21, 12389-12397 (2011).
194. W. H. Lee, J. Park, Y. Kim, K. S. Kim, B. H. Hong, and K. Cho, Control of graphene field-effect transistors by hydrophobic self-assembled monolayers, Adv. Mater. 23, 3460-3464 (2011).
195. Y. Cho, S. K. Min, W. Y. Kim, and K. S. Kim, The origin of dips for the graphene-based DNA sequencing device, Phys. Chem. Chem. Phys. 13, 14293-14296 (2011).
196. W. J. Cho, Y. Cho, S. K. Min, W. Y. Kim, and K. S. Kim, Chromium porphyrin arrays as spintronic devices, J. Am. Chem. Soc. 133, 9364-9369 (2011).
197. I. Geronimo, N. J. Singh, and K. S. Kim, Nature of anion-templated π+-π+ interactions, Phys. Chem. Chem. Phys. 13, 11841-11845 (2011).
198. S. Huh, J. Park, K. S. Kim, B. H. Hong, and S. B. Kim, Selective N-Type Doping of Graphene by Photo-Patterned Gold Nanoparticles, ACS Nano 5, 3639-3644 (2011).
199. F. Wang, X. Hong, J. Wang, K. S. Kim, Coordinate space translation technique for simulation of electronic process in the ion-atom collision, J. Chem. Phys. 134, 154308 (2011).
200. S. W. Heo, I.-C. Hwang, Y. Chun, J. W. Lee, N. J. Singh, S. Bin Kim, and K. S. Kim, Thermally Stable Intermolecular Proton Bonds in Polyaromatic Aldehyde Crystals, Chem. Asian J. 6, 2055-2061

(2011).

201. N. Ahmed, Inacrist Geronimo, I.-C. Hwang, N. Jiten Singh, K. S. Kim, cyclo-Bis(urea-3,6-dichlorocarbazole) as a Chromogenic and Fluorogenic Receptor for Anions and a Selective Sensor of Zinc and Copper Cations, Chem. Eur. J. 17, 8542-8548 (2011).
202. G. Lee, K. S. Kim, K. Cho, Theoretical Study of the Electron Transport in Graphene with Vacancy and Residual Oxygen Defects after High-Temperature Reduction, J. Phys. Chem. C 115, 9719-9725 (2011).
203. S. Myung, A. Solanki, C. Kim, J. Park, K. S. Kim, and K.-B. Lee, Graphene-Encapsulated Nanoparticle-Based Biosensor for the Selective Detection of Cancer Biomarkers. Adv. Mater. 23, 2221-2225 (2011).
204. H. M. Lee, D. Y. Kim, C. Pak, N. J. Singh, and K. S. Kim, H_2-Binding by Neutral and Multiply-Charged Titaniums: Hydrogen Storage Capacity of Titanium Mono- and Di-Cations**,** J. Chem. Theory Comput. 7, 969-978 (2011).
205. I. Geronimo, N. J. Singh, and K. S. Kim, Can Electron-rich π Systems Bind Anions? J. Chem. Theory Comput. 7, 825-829 (2011).
206. W. H. Lee, J. Park, S. H. Sim, S. B. Jo. K. S. Kim, B. H. Hong, and K. Cho, Transparent Flexible Organic Transistors based on Monolayer Graphene Electrodes on Plastic, Adv. Mater. 23, 1752-1756 (2011).
207. W. H. Lee, J. Park, S. H. Sim, S. Lim, K. S. Kim, B. H. Hong, and K. Cho, Surface-Directed Molecular Assembly of Pentacene on Monolayer Graphene for High-Performance Organic Transistors, J. Am. Chem. Soc. 133, 4447-4454 (2011).
208. J. Park, W. H. Lee, S. Huh, S. H. Sim, S. B. Kim, K. Cho, B. H. Hong, and K. S. Kim, Work-Function Engineering of Graphene Electrodes by Self-Assembled Monolayers for High-Performance Organic Field-Effect Transistors, J. Phys. Chem. Lett. 2, 841-845 (2011).
209. D. Y. Kim, H. M. Lee, S. K. Min, Y. Cho, I.-C. Hwang, K. Han, J. Y. Kim, and K. S. Kim*, CO_2 Capturing Mechanism in Aqueous Ammonia: NH_3-driven Decomposition-Recombination Pathway, J. Phys. Chem. Lett. 2, 689-694 (2011).
210. Y. Cho, Y. C. Choi, and K. S. Kim, Graphene Spin-Valve Device Grown Epitaxially on the Ni(111) Substrate: A First Principles Study, J. Phys. Chem. C. 115, 6019-6023 (2011).
211. V. Chandra and K. S. Kim, Highly Selective Adsorption of Hg2+ by Polypyrrole-Reduced Graphene Oxide Composite, Chem. Commun. 47, 3942-3944 (2011).
212. M. Guin, G. N. Patwari, S. Karthkeyan, K. S. Kim, Do N-Heterocyclic Aromatic Rings Prefer π–Stacking? Phys. Chem. Chem. Phys. 13, 5514-5525 (2011).
213. S. K. Min, W. Y. Kim, Y. Cho, K. S. Kim, Fast DNA sequencing with a graphene-based nanochannel device, **Nature Nanotech.** 6, 162-165 (2011).
214. N. J. Singh, D. Shin, H. M. Lee, H. T. Kim, H.-J. Chang, J. M. Cho, K. S. Kim, S. Ro, Structural Basis of Triclosan Resistance, J. Struct. Biol. 174, 173-179 (2011).
215. Z. Xu, N. J. Singh, S. K. Kim, D. R. Spring, K. S. Kim, J. Yoon, "Induction-driven stabilization of anion-pi interaction in electron rich aromatics as the key to the fluoride inclusion in cage-imidazolium receptors", Chem. Eur. J. 17, 1163-1170 (2011).
216. N. Kim, K. S. Kim, N. Jung, L. Brus, P. Kim, Synthesis and Electrical Characterization of Magnetic Bilayer Graphene Intercalate, Nano Lett. 11, 860-865 (2011).
217. J. W. Yi, J. Park, N. J. Singh, I. J. Lee, K. S. Kim, B. H. Kim, Quencher-free molecular beacon: Enhancement of the signal-to-background ratio with graphene oxide, Bioorg. Med. Chem. Lett. 21, 704-706 (2011).
218. M. Kolaski, A. Kumar, N. J. Singh and K. S. Kim, Differences in structure, energy, and spectrum between neutral, protonated, and deprotonated phenol dimers: Comparison of various density functionals with ab initio theory, Phys. Chem. Chem. Phys. 13, 991-1001 (2011).
219. V. Tipmanee, H. Oberhofer, M. Park, K. S. Kim, J. Blumberger, Prediction of reorganization free energies for biological electron transfer: A comparative study of Ru-modified cytochromes and a 4-helix bundle protein. J. Am. Chem. Soc. 132, 17032-17040 (2010).
220. S. Karthikeyan, H. M. Lee, K. S., Kim, Structure, Stabilities, Thermodynamic properties and IR

spectra of acetylene cluster (C2H2)n=2-5, J. Chem. Theory Comput. 6, 3190-3197 (2010).

221. E. C. Lee, Y. C. Choi, W. Y. Kim, N. J. Singh, S. Lee, J. H. Shim, K. S. Kim, A Radical Polymer as a Two-Dimensional Organic Half Metal, Chem. Eur. J. 16, 12141-12146 (2010).
222. S. K. Min, M. Park, N. J. Singh, H. M. Lee, E. C. Lee, K. S. Kim, A. Lagutschenkov, and G. Niedner-Schatteburg, Chiral transformation in protonated and deprotonated adipic acids through multi-step internal proton transfer, Chem. Eur. J. 16, 10373-10379 (2010).
223. S. Maity, A. Dey, G. N. Patwari, S. Karthikeyan, K. S. Kim, A Combined Spectroscopic and ab initio Investigation of Phenylacetylene-Methylamine Complex. Observation of σ and π Type Hydrogen-Bonded Configurations and Fluorescence Quenching by Weak C–H•••N Hydrogen Bonding, J. Phys. Chem. A 114, 11347-11352 (2010).
224. S. Bae, H. Kim, Y. Lee, X. Xu, J.-S. Park, Y. Zheng, J. Balakrishnan, T. Lei, H. R. Kim, Y. I. Song, Y.-J. Kim, K. S. Kim, B. Ozyilmaz, J.-H. Ahn, B. H. Hong and S. Iijima, Roll-to-roll production of 30-inch graphene films for transparent electrodes, **Nature Nanotech.** 5, 574-578 (2010).
225. V. Chandra, J. Park, Y. Chun, J. W. Lee, I.-C. Hwang, K. S. Kim, Water Dispersible Magnetite-Reduced Graphene Oxide Composites for Arsenic Removal, ACS Nano 4, 3979-3986 (2010).
226. I. Geronimo, E. C. Lee, N. J. Singh, and K. S. Kim, How Different are Electron-rich and Electron-deficient π Interactions?, J. Chem. Theory Comput. 6, 1931-1934 (2010).
227. D. R. Mason, D. K. Gramotnev, K. S. Kim, Wavelength-dependent transmission through sharp 90o bends in sub-wavelength metallic slot waveguides, Opt. Express 18, 16319-16145 (2010).
228. S. Han, N. J. Singh, T. Y. Kang, K.-W. Choi, S. Choi, S. J. Baek, K. S. Kim, and S. K. Kim, Aromatic pi-pi interaction mediated by a metal atom: structure and ionization of the bis(eta^6-benzene)chromium-benzene cluster, Phys. Chem. Chem. Phys., 12, 7648-7653 (2010).
229. D. R. Mason, M. V. Jouravlev, and K. S. Kim, Enhanced Resolution Beyond the Abbe Diffraction Limit with Wavelength Scale Solid Immersion Lenses, Opt. Lett. 35, 2007-2009 (2010).
230. S. Maity, G. N. Patwari, S. Karthikeyan, and K. S. Kim, Binary Complexes of Tertiary Amines with Phenylacetylene. Dispersion wins over Electrostatics, Phys. Chem. Chem. Phys. 12, 6150-6156 (2010).
231. I.-C. Hwang, S. W. Heo, N. J. Singh, J. W. Lee, Y. Chun, S. B. Baek, K. S. Jin, M. Ree, H. C. Lee, S. B. Kim, and K. S. Kim, Self-Assembled Thermally Highly Stable 1-Dimensional Proton Arrays, J. Phys. Chem. B 114, 7216-7221 (2010).
232. J. Wang, K. S. Kim, and E. J. Baerends, Counterintuitive Coulomb hole around the bond midplane, J. Chem. Phys. 132, 204102 (2010).
233. H. M. Lee, A. Kumar, M. Kolaski, D. Y. Kim, E. C. Lee, S. K. Min, M. Park, Y. C. Choi, and K. S. Kim, Comparison of Cationic, Anionic and Neutral Hydrogen Bonded Dimers, Phys. Chem. Chem. Phys. 12, 6278-6287 (2010).
234. A. Das, A. D. Jana, S. K. Seth, B. Dey, S. R. Choudhury, T. Kar, S. Mukhopadhyay, N. J. Singh, I.-C. Hwang, and K. S. Kim, Intriguing π^+ - π Interaction in Crystal Packing, J. Phys. Chem. B 114, 4166-4170 (2010).
235. D. Y. Kim, H. M. Lee, J. Seo, S. K. Shin, and K. S. Kim, Rules and Trends of Metal Cation Driven Hydride-Transfer Mechanisms in Metal Amidoboranes, Phys. Chem. Chem. Phys. 12, 5446-5453, (2010).
236. W. Y. Kim and K. S. Kim, Tuning Molecular Orbitals in Molecular Electronics and Spintronics, Acc. Chem. Res. 43, 111-120 (2010).
237. S. Myung, J. Park, H. Lee, K. S. Kim and S. Hong, Ambipolar Memory Devices based on Reduced Graphene Oxide and Nanoparticles, Adv. Mater. 22, 2045-2049 (2010).
238. S. M. Yoon, H. J. Song, I.-C. Hwang, K. S. Kim, and H. C. Choi, Single Crystal Structure of Copper Hexadecafluorophthalocyanine (F16CuPc) Ribbon, Chem. Commun. 46, 231-233 (2010).
239. J.-H. Choi, K. S. Kim, and J.-H. Cho, Antiferromagnetic spin ordering in the dissociative adsorption of H2 on Si(001): Density-functional calculations, J. Chem. Phys. 131, 244704 (2009).
240. M. Guin, G. N. Patwari, S. Karthikeyan, K. S. Kim, A pi-Stacked Phenylacetylene and 1,3,5-Triazine Hetero Dimer: A Combined Spectroscopic and Ab-initio investigation, Phys. Chem. Chem. Phys. 11, 11207-11212 (2009).

241. Z. Xu, N. J. Singh, J. Lim, J. Pan, H. N. Kim, S. Park, K. S. Kim, and J. Yoon, Unique Sandwich Stacking of Pyrene-Adenine-Pyrene for Selective and Ratiometric Fluorescent Sensing of ATP at Physiological pH, J. Am. Chem. Soc. 131, 15528-15533 (2009).
242. Y.-J. Yu, Y. Zhao, S. Ryu, L. E. Brus, K. S. Kim, and P. Kim, Tuning the graphene work function by electric field effect, Nano Lett. 9, 3430-3434 (2009).
243. J. Y. Lee, B. H. Hong, W. Y. Kim, S. K. Min, Y. Kim, M. V. Jouravlev, R. Bose, K. S. Kim, I.-C. Hwang, L. J. Kaufman, C. W. Wong, P. Kim, and K. S. Kim, Near-field focusing and magnification through self-assembled nanoscale spherical lenses, **Nature** 460, 498-501 (2009). *highlighted in Laser Focus World, NPG Asia Materials (Nature Publ. Group), Technology Review (MIT), Nature Nananotech., Chem. & Eng. News (Am. Chem. Soc.), Nanotechweb.org (IOP), and Korean TVs and newspapers.* (한국 과총 2009 10 선)
244. Y. Park, N. J. Singh, K. S. Kim, T. Tachikawa, T. Majima, and W. Choi, Fullerol-Titania Charge Transfer Mediated Photocatalysis Working under Visible Light, Chem. Eur. J. 15, 10843-10850 (2009).
245. K. S. Kim, Y. Zhao, H. Jang, S. Y. Lee, J. M. Kim, K. S. Kim, J.-H. Ahn, P. Kim, J.-Y. Choi, and B. H. Hong, Large-scale pattern growth of graphene films for stretchable transparent electrodes, **Nature** 457, 706-710 (2009). *Highlighted in New York Times.*
246. W. Y. Kim, Y. C. Choi, S. K. Min, Y. Cho, and K. S. Kim, Application of quantum chemistry to nanotechnology: electron/spin transport in molecular devices, Chem. Soc. Rev. 38, 2319-2333 (2009).
247. S. Karthikeyan and K. S. Kim, Structure, Stability, Thermodynamic Properties and IR Spectra of the Protonated Water Decamer H+(H2O)10, J. Phys. Chem. A 113, 9237-9242 (2009).
248. H.-B. Yi, H. M. Lee, K. S. Kim, Interaction of benzene with transition metal cations: Theoretical Study of structures, energies, and IR spectra, J. Chem. Theor. Comput. 5, 1709-1717 (2009).
249. D. Y. Kim, N. J. Singh, H. M. Lee, and K. S. Kim, Hydrogen Release Mechanisms in Lithium Amidoboranes, Chem. Eur. J. 15, 5598-5604 (2009).
250. J.-Y. Park, Y.-S. Lee, B.-Y. Chang, S. Karthikeyan, K. S. Kim, B. H. Kim, and S.-M. Park, R)-Lipo-Diaza-18-Crown-6 Self-Assembled Monolayer as a Selective Serotonin Receptor, Anal. Chem. 81, 3843-3850 (2009).
251. I.-C. Hwang, R. Kumar, N. D. Kim, Y. Chun, J. W. Lee, P. Kumar, R. S. Mana, C. Choi, J. R. Lee, and K. S. Kim, Controlling metal nanotoppings on the tip of silicide nanostructures, Nanotech. 20, 245605 (2009).
252. S. Karthikeyan and K. S. Kim, Structure, Stability, Thermodynamic Properties and IR Spectra of the Protonated Water Cluster H+(H2O)9, Mol. Phys. 107, 1169-1176 (2009).
253. Y. C. Choi, W. Y. Kim, H. M. Lee, and K. S. Kim, Neutral and Anionic Gold Decamers: Planar Structure with Unusual Spatial Charge-Spin Separation, J. Chem. Theor. Comput. 5, 1216-1223 (2009).
254. Y. Cho, W. Y. Kim, and K. S. Kim, Effect of electrodes on electronic transport of molecular electronic devices, J. Phys. Chem. A 113, 4100-4104 (2009).
255. H. M. Lee and K. S. Kim, Water Dimer Cation: Density Functional Theory vs Ab Initio Theory, J. Chem. Theor. Comput. 5, 976-981 (2009).
256. S. M. Yoon, I.-C. Hwang, K. S. Kim, H. C. Choi, Synthesis of Single Crystal Tetra(4-pyridyl)porphyrin Rectangular Nanotubes in the Vapor Phase, Angew. Chem. Int. Ed. 48, 2506-2509 (2009).
257. H. M. Lee, D. J. Anick, and K. S. Kim, Structures of Tri-, Tetra-, and Hexahydrated Hydride Anion Clusters, Int. J. Quant. Chem. 109, 1820-1826 (2009).
258. N. J. Singh, S. K. Min, D. Y. Kim, and K. S. Kim, Comprehensive Energy Analysis for Various Types of pi-Interaction, J. Chem. Theor. Comput. 5, 515-529 (2009).
259. W. Y. Kim, Y. C. Choi, and K. S. Kim, Understanding structures and electronic/spintronic properties of single molecules, nanowires, nanotubes, and nanoribbons toward the design of nanodevices, J. Mater. Chem. (feature article). 18, 4510-4521 (2008).
260. S. Karthikeyan, M. Park, I. Shin, and K. S. Kim, Structure, Stability, Thermodynamic properties and infrared spectra of the protonated water octamer H+(H2O)8, J. Phys. Chem. A 112, 10120-10124 (2008).

261. W. Y. Kim and K. S. Kim, Prediction of very large values of magnetoresistance in a graphene nanoribbon device, **Nature Nanotech.** 3, 408-412 (2008). *Highlighted in NPG Asia materials.*
262. D. Y. Kim, N. J. Singh, and K. S. Kim, Cyameluric Acid as anion-pi type receptor for ClO4- and NO3-: pi-stacked and edge-to-face structures, J. Chem. Theor. Comput. 4, 1401-1407 (2008).
263. D. Y. Kim, N. J. Singh, J. W. Lee, and K. S. Kim, Solvent driven structural changes in anion-π complexes, J. Chem. Theor. Comput. 4, 1162-1169 (2008).
264. S. Karthikeyan, J. N. Singh, M. Park, R. Kumar, and K. S. Kim, Structures, energetics, vibrational spectra of NH4+(H2O)n=4,6 clusters: ab initio calculations and first principles molecular dynamics simulations, J. Chem. Phys. 128, 244304 (2008).
265. S. Karthikeyan, J. N. Singh, and K. S. Kim, Undissociated vs. dissociated structures for water clusters and ammonia-water clusters: (H2O)n and NH3(H2O)n-1 (n=5,8,9,21): Theoretical Study, J. Phys. Chem. A 112, 6527-6532 (2008).
266. Wang and K. S. Kim, Large-scale polyol synthesis of single crystal bismuth nanowires and the role of NaOH in the synthesis process, Nanotech. 19, 265303 (2008).
267. A. Kumar, M. Kołaski, H. M. Lee, and K. S. Kim, Photo-excitation and photo-ionization dynamics of water photolysis, J. Phys. Chem. A 112, 5502-5508 (2008).
268. H. M. Lee and K. S. Kim, Hydrogen detachment of the hydrated hydro-halogen acids upon attaching an excess electron, J. Chem. Phys. 128, 104310 (2008).
269. H. M. Lee, M. Kolaski, and K. S. Kim, Photo-dissociation of hydrated hydrogen iodide clusters, ChemPhysChem 9, 567-571 (2008).
270. S. K. Min, E. C. Lee, H. M. Lee, D. Y. Kim, D. Kim, and K. S. Kim, Complete Basis Set Limit of Ab Initio Binding Energies and Geometrical Parameters for Various Typical Types of Complexes, J. Comput. Chem. 29, 1208-1221 (2008).
271. W. Y. Kim and K. S. Kim, Carbon nanotube, graphene, nanowire, and molecule-based electron and spin transport phenomena using the non-equilibrium Green function method at the level of first principles theory, J. Comput. Chem. 29, 1073-1083 (2008).
272. Y. K. Kim, H. N. Lee, N. J. Singh, H. J. Choi, J. Y. Xue, K. S. Kim, J. Yoon, and M. H. Hyun, Anthracene Derivatives Bearing Thiourea and Glucopyranosyl Groups for the Highly Selective Chiral Recognition of Amino Acids: Opposite Chiral Selectivities from Similar Binding Units, J. Org. Chem. 73, 301-304 (2008).
273. A. Kumar, M. Kołaski, and K. S. Kim, Ground state structures and excited state dynamics of pyrrole-water complexes: ab initio excited state molecular dynamics simulations, J. Chem. Phys. 128, 034304 (2008).
274. M. Kolaski, H. M. Lee, C. Pak, and K. S. Kim, Charge-transfer-to-solvent-driven dissolution dynamics of I-$(H2O)_{2-5}$ upon excitation: excited-state ab initio molecular dynamics simulations, J. Am. Chem. Soc. 130, 103-112 (2008).
275. M. Diefenbach and K. S. Kim, Towards molecular magnetic switching with an electric bias, Angew. Chem. Int. Ed. 46, 7640-7643 (2007); Angew. Chem. 119, 7784-7787 (2007).
276. S. Shim, I. Eom, T. Joo, E. Kim, and K. S. Kim, Ring Closure Reaction Dynamics of Diarylethene Derivatives in Solution, J. Phys. Chem. A 111, 8910-8917 (2007).
277. H. M. Lee, D. Kim, N. J. Singh, M. Kolaski, and K. S. Kim, Hydrated hydride anion clusters, J. Chem. Phys. 127, 164311 (2007).
278. M. Park, I. Shin, N. J. Singh, and K. S. Kim, Eigen and Zundel forms of small protonated water clusters: structures and infrared spectra, J. Phys. Chem. A 111, 10692-10702 (2007).
279. H. M. Lee, S. Odde, B. J. Mhin, S. B. Suh, and K. S. Kim, Hydrogen detachment of the hexa-hydrated hydro-iodic acid upon attaching an excess electron, Mol. Phys. 105, 2577-2581 (2007).
280. D. Kim, E. C. Lee, K. S. Kim, and P. Tarakeshwar, Cation-pi-anion interaction: A theoretical investigation of the role of induction energies, J. Phys. Chem. A 111, 7980-7986 (2007).
281. W. Y. Kim, S. K. Kwon, and K. S. Kim, Negative Differential Resistance of Carbon Nanotube Electrodes with Asymmetric Coupling Phenomena, Phys. Rev. B 76, 033415 (2007).
282. Y. Wang, J. Y. Lee, J.-S. Kim, G. H. Kim, and K. S. Kim, Diameter- and Length-Dependent Volume

Plasmon Excitation of Bismuth Nanorods Investigated by Electron Energy Loss Spectroscopy, Chem. Mat. 19, 3912-3916 (2007).

283. T. D. Thangadurai, N. J. Singh, I.-C. Hwang, J. W. Lee, R. P. Chandran, and K. S. Kim, 2-Dimensional Analytic Approach for Anion Differentiation with Chromo-Fluorogenic Receptors, J. Org. Chem. 72, 5461-5464 (2007).
284. E. C. Lee, D. Kim, P. Jurečka, P. Tarakeshwar, P. Hobza, and K. S. Kim, Understanding of Assembly Phenomena by Aromatic-aromatic interactions: benzene dimer and the substituted systems, J. Phys. Chem. A 111, 3446-3457 (2007). (Feature Article).
285. N. Jiten Singh, Han Myoung Lee, In-Chul Hwang, and Kwang S. Kim, Designing Ionophores and Molecular Nanotubes Based on Molecular Recognition, Supramol. Chem. 19, 321-332 (2007). (Review Article).
286. N. J. Singh, E. C. Lee, Y. C. Choi, H. M. Lee, K. S. Kim, Understanding Clusters toward the Design of Functional Molecules and Nanomaterials, Bull. Chem. Soc. Japan, 80, 1437-1450 (2007). (Commemorative Accounts).
287. A. C. Olleta, H. M. Lee, and K. S. Kim , Ab initio study of hydrated potassium halides KX(H2O)1-6 (X=F, Cl, Br, I), J. Chem. Phys. 126, 144311 (2007).
288. N. J. Singh, H. M. Lee, S. B. Suh and K. S. Kim, De novo design approach based on nanorecognition toward development of functional molecules/materials and nanosensors/nanodevices, Pure Appl. Chem. 79, 1057-1075 (2007).
289. S. J. Youn, T. H. Rho, B. I. Min, and K. S. Kim, Extended Drude model analysis of noble metals, Phys. Stat. Sol. (b), 244, 1354-1362 (2007).
290. J. S. Kim, J. H. Jung, S. J. Lee, I.-C. Hwang, N. J. Singh, S. K. Kim, S. H. Lee, H. J. Kim, C. S. Keum, J. W. Lee, and K. S. Kim, A color version of the Hinsberg test: 1^{o}–3^{o} amine indicator, Chem. Eur. J. 13, 3082-3088 (2007).
291. J.-S. Wu, I.-C. Hwang, K. S. Kim, and J. S. Kim, Rhodamine-Based Hg_2^{+}-Selective Chemodosimeter in Aqueous Solution: Fluorescent OFF-ON, Org. Lett. 9, 907-910 (2007).
292. Y. C. Choi, H. M. Lee, W. Y. Kim, S. K. Kwon, T. Nautiyal, D.-Y. Cheng, K. Vishwanathan, and K. S. Kim, How can we make stable linear monoatomic chains? gold-cesium binary subnanowires as an example of charge-transfer-driven approach to alloying, Phys. Rev. Lett. 98, 076101 (2007).
293. M. Kolaski, H. M. Lee, Y. C. Choi, K. S. Kim, P. Tarakeshwar, D. J. Miller, and J. M. Lisy, Structures, energetics, and spectra of aqua-cesium(I) complexes: An ab initio and experimental study, J. Chem. Phys. 126, 074302 (2007).
294. H. N. Lee, N. J. Singh, S. K. Kim, J. Y. Kwon, Y. Y. Kim, K. S. Kim and J. Yoon, New imidazolium systems bearing two pyrene groups as fluorescent chemosensors for anions and anion induced logic gates, Tetrahedron Lett., 48, 169-172 (2007).
295. N. J. Singh, E. J. Jun, K. Chellappan, D. Thangadurai, R. P. Chandran, I.-C. Hwang, J. Yoon, K. S. Kim, Quinoxaline-Imidazolium Receptors for Unique Sensing of Pyrophosphate and Acetate by Charge Transfer, Org. Lett. 9, 485-488 (2007).
296. A. Bala, T. Nautiyal, and K. S. Kim, Effect of dimensionality on transition-metal elements of groups 3-7, Phys. Rev. B 74, 174429(1-5) (2006).
297. I. Shin, M. Park, S. K. Min, E. C. Lee, S. B. Suh, and K. S. Kim, Structure and spectral features of H+(H2O)7: Eigen vs. Zundel forms, J. Chem. Phys.125, 234305 (2006).
298. I.-C. Hwang, R. P. Chandran,, N. J. Singh; M. Khandelwal, T. D. Thangadurai, J.-W. Lee, J. A. Chang, and K. S. Kim, Organic-Inorganic Hybrid Compounds of Li with Bisimidazole Derivatives: Li Ion Binding Study and Topochemical Properties, Inorg. Chem. 45, 8062-8069 (2006).
299. S. K. Kim, N. J. Singh, J. Kwon, I.-C. Hwang, S. J. Park, K. S. Kim, and J. Yoon, Fluorescent imidazolium receptors for the recognition of pyrophosphate, Tetrahedron 62, 6065-6072 (2006).
300. A. Kumar, M. Park, J. Y. Huh, H. M. Lee, and K. S. Kim, Hydration phenomena of sodium and potassium hydroxides by water molecules" J. Phys. Chem. A 110, 12484-12493 (2006).
301. H.-B. Yi, H. M. Lee, S. B. Suh, S. K. Shin, and K. S. Kim, Pseudorotation-driven dynamical structure of the tropyl radical, J. Chem. Phys. 125, 164332 (2006).

302. M. Diefenbach and K. S. Kim, Spatial structure of Au8: Importance of basis set completeness and geometry relaxation, J. Phys. Chem. B 110, 21639-21642 (2006).
303. H. Zhou, N. J. Singh, and K. S. Kim, Homology modeling and molecular dynamics study of west nile virus NS3 protease: A molecular basis for the catalytic activity increased by the NS2B cofactor, Proteins: Structure, Function, and Bioinformatics, 65, 692-701 (2006).
304. Y. W. Wang, J. S. Kim, G. H. Kim, and K. S. Kim, Quantum size effects in the volume plasmon excitation of bismuth nanoparticles investigated by electron energy loss spectroscopy, Appl. Phys. Lett. 88, 143106/1-3 (2006).
305. J. Yoon, S. K. Kim, N. J. Singh and K. S. Kim, Imidazolium Receptors for the Recognition of Anions, Chem. Soc. Rev. 35, 355-360 (2006).
306. H.-B. Yi, M. Diefenbach, Y. C. Choi, E. C. Lee, H. M. Lee, B. H. Hong, and K. S. Kim, Interactions of Neutral and Cationic Transition Metals with the Redox System of Hydroquinone and Quinone: Theoretical Characterization of the Binding Topologies, and Implications for the Formation of Nanomaterials, Chem. Eur. J. 12, 4885-4892 (2006).
307. N. J. Singh, M. Park, S. K. Min, S. B. Suh, and K. S. Kim, Magic and anti-magic protonated water clusters: Exotic structures with unusual dynamic effects, Angew. Chem. Int. Ed. 45, 3795-3800 (2006); Angew. Chem. 118, 3879-3884 (2006).
308. S. Odde, B. J. Mhin, K. H. Lee, H. M. Lee, P. Tarakeshwar, and K. S. Kim, Hydration and dissociation of hydrogen fluoric acid (HF), J. Phys. Chem. A 110, 7918-7924 (2006).
309. H. Zhou, N. J. Singh, and K. S. Kim, Homology Modeling and Molecular Dynamics Study of Chorismate Synthase from Shigella Flexneri, J. Mol. Graphics & Modeling, 25, 434-441 (2006).
310. S. Vaupel, B. Brutschy, P. Tarakeshwar, and K. S. Kim, Characterization of Weak NH-pi Intermolecular Interactions of Ammonia with Various Substituted pi Systems, J. Am. Chem. Soc. 128, 5416-5426 (2006).
311. D. Cheng, W. Y. Kim, S. K. Min, T. Nautiyal, and K. S. Kim, Magic structures and Quantum Conductance of [110] silver nanowires, Phys. Rev. Lett. 96, 096104/1-4 (2006).
312. Y.C. Choi, C. Pak, and K. S. Kim, Electric field effects on water clusters (n=3-5): Systematic ab initio study of structures, energetics, and transition states, J. Chem. Phys. 124, 094308/1-4 (2006).
313. N. J. Singh, H.-B. Yi, S. K. Min, M. Park, and K. S. Kim, Dissolution Nature of Cesium Fluoride by Water Molecules, J. Phys. Chem. B 110, 3808-3815 (2006).
314. N. J. Singh, A. C. Olleta, A. Kumar, M. Park, H.–B. Yi, I. Bandyopadhyay, H. M. Lee, P. Tarakeshwar, and K. S. Kim, Study of Interactions of Various Ionic Species with Solvents Towards the Design of Receptors, Theor. Chem. Acc.115, 127-135 (2006).
315. A. C. Olleta, H. M. Lee, and K. S. Kim, Ab initio study of hydrated sodium halides NaX(H2O)1-6 (X = F, Cl, Br, and I), J. Chem. Phys. 124, 024321 (2006).
316. J-H. Cho, K. S. Kim, Y. Morikawa, Structure and binding energies of unsaturated hydrocarbons on Si(001) and Ge(001), J. Chem. Phys. 124, 024716/1-4 (2006).
317. B. H. Hong, J. P. Small, M. S. Purewal, A. Mullokandov, M. Y. Sfeir, F. Wang, J. Y. Lee, T. F. Heinz, L. E. Brus, P. Kim, and K. S. Kim, Extracting Subnanometer Single Shells from Ultralong Multi-Walled Carbon Nanotubes, Proc. Nat. Acad. Sci. USA. 102, 14155-14158 (2005). *Highlighted in Nature (Materials website).*
318. B. H. Hong, J. Y. Lee, T. Beetz, Y. Zhu, P. Kim, and K. S. Kim, Quasi-Continuous Growth of Ultralong Carbon Nanotube Arrays, J. Am. Chem. Soc. 127, 15336-15337 (2005).
319. M. Kolaski, H. M. Lee, C. Pak, M. Dupuis, and K. S. Kim, Ab initio molecular dynamics simulations of an excited state of X-(H2O)3 (X=Cl, I) complex, J. Phys. Chem. A 109, 9419-9423 (2005).
320. S. K. Kwon, B. I. Min, S. J. Youn, and K. S. Kim, Electronic structures of diboride compounds: AgB2 and AuB2. J. Korean Phy. Soc. 46, L1295-1298 (2005).
321. Y. J. Kim, Y. A. Kim, N. Park, H. S. Son, K. S. Kim, and J. H. Hahn, Structural Characterization of the Molten Globule State of Apomyoglobin by Limited Proteolysis and HPLC-Mass Spectrometry, Biochemistry 44, 7490-7496 (2005).
322. A. Veerman, H. M. Lee, and K. S. Kim, Dissolution nature of the lithium hydroxide by water

molecules, J. Chem. Phys. 123, 084321 (2005).

323. H. M. Lee, M. Diefenbach, S. B. Suh, P. Tarakeshwar, and K. S. Kim, Why the hydration energy of Au+ is larger for the second water molecule than the first one: Skewed Orbitals Overlap, J. Chem. Phys. 123, 074328 (2005).
324. S. K. Kim, N. J. Singh, S. J. Kim, K. M. K. Swamy, S. H. Kim, K.-H. Lee, K. S. Kim, and J. Yoon, Anthracene Derivatives Bearing two urea groups as Fluorescent Receptors for Anions, Tetrahedron, 61, 4545-4550 (2005).
325. K. Chellappan, N. J. Singh, I.-C. Hwang, J. W. Lee, and K. S. Kim, A Calix[4]imidazolium[2]pyridine as an Anion Receptor, Angew. Chem. Int. Ed. 44, 2899-2903 (2005); Angew. Chem. 117, 2959 (2005).
326. E. C. Lee, B. H. Hong, J. Y. Lee, J. C. Kim, D. Kim, Y. Kim, P. Tarakeshwar, and K. S. Kim, Substituent Effects on the Edge-to-Face Aromatic Interactions, J. Am. Chem. Soc. 127, 4530-4537 (2005).
327. Y. C. Choi, W. Y. Kim, K.-S. Park, P. Tarakeshwar, K. S. Kim, T.-S. Kim, and J. Y. Lee, Role of molecular orbitals of the benzene in electronic nano-devices, J. Chem. Phys. 122, 094706 (2005).
328. W. Y. Kim, T. Nautiyal, S. J. Youn, and K. S. Kim, Anomalous behavior of mercury in one-dimension: Density functional calculations, Phys. Rev. B 71, 113104 (2005).
329. Y. W. Wang, B. H. Hong, and K. S. Kim, Size Control of Semimetal Bismuth Nanoparticles and the UV-Visible and IR Absorption Spectra, J. Phys. Chem. B 109, 7067-7072 (2005).
330. T. K. Manojkumar, S. B. Suh, K. S. Oh, S. J. Cho, C. Cui, X. Zhang, K. S. Kim, Theoretical Studies on the Mechanism of Acid Promoted Hydrolysis of N-Formylaziridine in Comparison with Formamide, J. Org. Chem. 70, 2651-2659 (2005).
331. T. K. Manojkumar, C. Cui, and K. S. Kim, Theoretical insights into the mechanism of acetylcholinesterase-catalyzed acylation of acetylcholine, J. Comput. Chem. 26, 606-611 (2005).
332. H. M. Lee, S. K. Min, E. C. Lee, J. H. Min, S. Odde, and K. S. Kim, Hydrated copper and gold mono-valent cations: Ab initio study, J. Chem. Phys. 122, 064314 (2005).
333. I. Bandyopadhyay, H. M. Lee, and K. S. Kim, Phenol vs. Water Molecule Interacting with Various Molecules: σ-Type, π-Type, and χ-Type Hydrogen Bonds, Interaction Energies and their Energy Components, J. Phys. Chem. A 109, 1720-1728 (2005).
334. H. M. Lee, S. B. Suh, P. Tarakeshwar, and K. S. Kim, Origin of the magic numbers of water clusters with an excess electron, J. Chem. Phys. 122, 044309 (2005).
335. C. Pak, H. M. Lee, J. C. Kim, D. Kim, K. S. Kim, Theoretical Investigation of Normal to Strong Hydrogen Bonds, Struct. Chem. 16, 187-202 (2005).
336. T. K. Manojkumar, D. Kim, and K. S. Kim, Theoretical studies on hydroquinone-benzene clusters, J. Chem. Phys. 122, 014305-5 (2005).
337. S. Odde, B. J. Mhin, H. M. Lee, and K. S. Kim, HF(H2O)n clusters with an excess electron: Ab initio study, J. Chem. Phys. 121, 11083-11087, (2004).
338. Y. W. Wang, B. H. Hong, J. Y. Lee, J.-S. Kim, G. H. Kim, and K. S. Kim, Antimony Nanowires Self-Assembled from Sb Nanoparticles, J. Phys. Chem. B, 108, 16723-16726, (2004).
339. A. V. Goncharenko, M. M. Dvoynenko, V. Z. Lozovski, and K. S. Kim. Local-field enhancement of spontaneous decay in nanosystems: some estimations for dielectric particles, Appl. Phys. B 79, 863-870 (2004).
340. J. Y. Kwon, N. J. Singh, N. H. Kim, S. K. Kim, K. S. Kim, and J. Yoon, Fluorescent GTP-sensing in Aqueous Solution of Physiological pH, J. Am. Chem. Soc. 126, 8892-8893 (2004).
341. H. M. Lee and K. S. Kim, Solvent rearrangement for an excited electron of the iodide-water pentamer, Mol. Phys. 102, 23/24, 2485-2489 (2004).
342. S. Odde, H. M. Lee, M. Kolaski, B. J. Mhin, and K. S. Kim, Dissolution of a base (RbOH) by water clusters, J. Chem. Phys., 121, 4665-4670 (2004).
343. H. M. Lee, P. Tarakeshwar, and K. S. Kim, Structures, energetics, and spectra of hydrated hydroxide anion clusters, J. Chem. Phys. 121, 4657-4664 (2004).
344. S. J. Lee, H. Y. Chung, and K. S. Kim, An easy-to-use three-dimensional molecular visualization and analysis program: POSMOL, Bull. Korean Chem. Soc. 25, 1061-1064 (2004).

345. T. K. Manojkumar, H. S. Choi, B. H. Hong, P. Tarakeshwar, and K. S. Kim, p-benzoquinone-benzene clusters as potential nanomechanical devices: A theoretical study, J. Chem. Phys. 121, 841-846 (2004).
346. S. Odde, C. Pak, H. M. Lee, K. S. Kim, and B. J. Mhin, Aqua dissociation nature of cesium hydroxide, J. Chem. Phys. 121, 204-208 (2004).
347. J. Park, M. Kolaski, H. M. Lee, and K. S. Kim, Insights into the structures, energetics, and vibrations of aqua-rubidium(l) complexes: Ab Initio study, J. Chem. Phys. 121, 3108-3116 (2004).
348. J. M. Park, J.-H. Cho, and K. S. Kim, Atomic Structure and energetics of adsorbed water on the NaCl(001) Surface, Phys. Rev. B 69, 233403 (2004).
349. T. Nautiyal, T. H. Rho, and K. S. Kim, Nanowires for spintronics: A study of transition-metal elements of groups 8-10, Phys. Rev. B 69, 193404 (2004).
350. J.-H. Cho and K. S. Kim, Metastable phase of symmetric dimers on Si(001), Phys. Rev. B 69, 125312 (2004).
351. S. Odde, B. J. Mhin, S. Lee, H. M. Lee, and K. S. Kim, Dissociation chemistry of hydrogen halides in water, J. Chem. Phys. 120, 9524-9535 (2004).
352. A. Hoffmann, D. Sebastiani, E. Sugiono, S. Yun, K. S. Kim, H. W. Spiess, and I. Schnell, Solvent molecules trapped in supramolecular organic nanotubes: a combined solid-state NMR and DFT study, Chem. Phys. Lett. 388, 164-169 (2004).
353. Y.-O. Kim, Y. M. Jung, S. B. Kim, B. H. Hong, K. S. Kim, and S.-M. Park, Mechanistic Study on Electrochemical Reduction of Calix[4]quinone in Acetonitrile Containing Water, J. Phys. Chem. B 108, 4927-4936 (2004).
354. H. M. Lee, P. Tarakeshwar, J. W. Park, M. R. Kolaski, Y. J. Yoon, H.-B. Yi, W. Y. Kim, and K. S. Kim, Insights into the structures, energetics, and vibrations of monovalent cation-(water)1-6 clusters, J. Phys. Chem. A 108, 2949-2958 (2004).
355. S. J. Youn, B. I. Min, T. H. Rho, and K. S. Kim, Nested Fermi surfaces, optical peaks, and laser-induced structural transition in Al, Phys. Rev. B 69, 033101 (2004).
356. W. T. Geng and K. S. Kim, Interplay of local structure and magnetism in Co-doped TiO2 anastase, Solid State Commun. 129, 741-746 (2004).
357. S. B. Suh, J. C. Kim, Y. C. Choi, and K. S. Kim, Nature of One-Dimensional Short Hydrogen Bonding: Bond Distances, Bond Energies, and Solvent Effects, J. Am. Chem. Soc. 126, 2186-2193 (2004).
358. D. Kim, P. Tarakeshwar, and K. S. Kim, Theoretical investigations of anion-π interactions: The role of anions and the nature of π systems, J. Phys. Chem. A 108, 1250-1258 (2004).
359. J. Yoon, S. K. Kim, N. J. Singh, J. W. Lee, Y. J. Yang, K. Chellappan, and K. S. Kim, Highly Effective Fluorescent Sensor for H2PO4-, J. Org. Chem. 69, 581-583 (2004).
360. C. Riehn, V. V. Matylitsky, W. Jareba, B. Brutschy, P. Tarakeshwar, and K. S. Kim, Insights into the Structure of Cyclohexane from Femtosecond Degenerate Four-wave Mixing Spectroscopy and Ab initio Calculations, J. Am. Chem. Soc. 125, 16455-16462 (2003).
361. H.-B. Yi, X.-H. Duan, J. Y. Lee, H. M. Lee, X.-Y. Li, and K. S. Kim, Theoretical study of photoinduced electron transfer from tetramethylethylene to tetracyanoethylene, J. Chem. Phys. 119, 8854-8863 (2003).
362. W.-T. Geng, and K. S. Kim, Structural, electronic, and magnetic properties of a ferromagnetic semiconductor: Co-doped TiO2 rutile, Phys. Rev. B 68, 125203 (2003).
363. H. M. Lee, S. B. Suh, and K. S. Kim, Solvent rearrangement for an excited electron of I-(H2O)6: Analog to structural rearrangement of e-(H2O)6, J. Chem. Phys. 119, 7685-7692 (2003).
364. E. C. Lee, H. M. Lee, P. Tarakeshwar, and K. S. Kim, Structures, energies, and spectra of aqua-silver(I) complexes, J. Chem. Phys. 119, 7725-7736 (2003).
365. J. Y. Lee, B. J. Mhin, S. Mukamel, and K. S. Kim, Size scaling of intramolecular charge transfer driven optical properties of substituted polyenes and polyynes, J. Chem. Phys. 119, 7519-7524 (2003).
366. H. M. Lee, M. Ge, B. R. Sahu, P. Tarakeshwar, and K. S. Kim, Geometrical and electronic structures of gold, silver, and gold-silver binary clusters: Origins of ductility of gold and gold-silver alloy formation, J. Phys. Chem. B 107, 9994-10005 (2003).
367. I. Bandyopadhyay, H. M. Lee, P. Tarakeshwar, C. Cui, K. S. Oh, J. Chin, and K. S. Kim, Highly

stereospecific epimerization of α-amino acids: Conducted tour mechanism, J. Org. Chem. 68, 6571-6575 (2003).

368. A. D. Reddy, S. B. Suh, R. Ghaffari, N. J. Singh, D.-J. Kim, J. H. Han, and K. S. Kim, Bioinformatics analysis of SARS proteins and molecular dynamics simulated structure of an alpha-helix motif, Bull. Korean Chem. Soc. 24, 899-900 (2003).
369. S. K. Kim, N. J. Singh, S. J. Kim, H. G. Kim, J. K. Kim, J. W. Lee, K. S. Kim, and J. Yoon, New fluoroscent photoinduced electron transfer chemosensor for the recognition of H2PO4- , Org. Lett. 5, 2083-2086 (2003).
370. T. Nautiyal, S. J. Youn, and K. S. Kim, Effect of dimensionality on the electronic structure of Cu, Ag, and Au, Phys. Rev. B 68, 033407 (2003).
371. W.-T. Geng, and K. S. Kim, Linear monatomic wires stabilized by alloying: Ab initio density functional calculations, Phys. Rev. B 67, 233403 (2003).
372. H. M. Lee, S. Lee, and K. S. Kim, Structures, energetics and spectra of electron-water clusters, e(-)-(H2O)2-6 and e(-)-HOD(D2O)1-5, J. Chem. Phys. 119, 187-194 (2003).
373. S. Shim, T. Joo, S. C. Bae, K. S. Kim, and E. Kim, Ring Opening Dynamics of a Photochromic Diarylethene Derivative in Solution, J. Phys. Chem. A 107, 8106-8110 (2003).
374. S. B. Suh, B. H. Hong, P. Tarakeshwar, S. J. Youn, S. Jeong, and K. S. Kim, Electronic Structure of Silver Subnanowires in Self-Assembled Organic Nanotubes: Density Functional Calculations, Phys. Rev. B (Rapid Commun.) 67, 241402(R) (2003).
375. S. Kim, From gas phase clusters to nanomaterials: An overview of theoretical insights, Bull. Korean Chem. Soc. 24, 757-762 (2003), Proceedings volume of the "Xth Korea-Japan Symposium on Theoretical/Computational Chemistry".
376. T. K. Manojkumar, H. S. Choi, P. Tarakeshwar, and K. S. Kim, Ab initio studies of neutral and anionic p-Benzoquinone-water clusters, J. Chem. Phys. 118, 8681-8686 (2003).
377. H. M. Lee, S. B. Suh, and K. S. Kim, Water heptamer with an excess electron: Ab initio study, J. Chem. Phys. 118, 9981-9986 (2003).
378. Y. Lee, B. J. Mhin, and K. S. Kim, New Quantum Chemical Parameter for the Substituent Effect in Benzene Based on Charge Flux, J. Phys. Chem. A 107, 3577-3579 (2003).
379. S. Yun, H. lhm, H. G. Kim, C.-W. Lee, B. Indrajit, K. S. Oh, Y. J. Gong, J. W. Lee, J. Yoon, H. C. Lee, and K. S. Kim, Molecular Recognition of Fluoride Anion: Benzene-Based Tripodal Imidazolium Receptor, J. Org. Chem. 68, 2467-2470 (2003).
380. S. Yun, Y. -O. Kim, D. Kim, H. G. Kim, H. lhm, J. K. Kim, C.-W. Lee, W. J. Lee, J. Yoon, K. S. Oh, J. Yoon, S.-M. Park, and K. S. Kim, Rational Design of Biologically Important Chemosensors: A Novel Receptor for Selective Recognition of Acetylcholine over Ammonium Cations, Org. Lett. 5, 471-474 (2003).
381. D. Kim, S. Hu, P. Tarakeshwar, K. S. Kim, and J. M. Lisy, Cation-π Interactions: A Theoretical Investigation of the Interaction of Metallic and Organic Cations with Alkenes, Arenes, and Heteroarenes, J. Phys. Chem. A 107, 1228-1238 (2003).
382. K. S. Kim, S. B. Suh, J. C. Kim, B. H. Hong, E. C. Lee, S. Yun, P. Tarakeshwar, J. Y. Lee, Y. Kim, H. Ihm, H. G. Kim, J. W. Lee, J. K. Kim, H. M. Lee, D. Kim, C. Cui, S. J. Youn, H. Y. Chung, H. S. Choi, C.-W. Lee, S. J. Cho, S. Jeong, and J.-H. Cho, Assembling phenomena of calix[4]hydroquinone nanotube bundles by one-dimensional short hydrogen bonding and displaced π-π stacking, J. Am. Chem. Soc. 124, 14268-14279 (2002).
383. H. G. Kim, C.-W. Lee, S. Yun, B. H. Hong, Y.-O. Kim, D. Kim, H. Ihm, J. W. Lee, E. C. Lee, P. Tarakeshwar, S.-M. Park, and K. S. Kim, "An Electrochemically Controllable Nanomechanical Molecular System Utilizing Edge-to-face and Face-to -face Aromatic Interacions", Org. Lett. 4, 3971-3974 (2002).
384. K. H. Kim, Y. S. Lee, D. Kim, K. S. Kim, and G.-H. Jeung, "Theoretical study of the gas phase Sc + (NO, O2) ® ScO + (N, O) reactions", J. Phys. Chem. A 106, 9600-9605 (2002).
385. P. Tarakeshwar and K.S. Kim, "Comparison of the nature of π and conventional H-bonds : a theoretical investigation", J. Mol. Str. 615, 227-238 (2002), Proceedings volume of the "XIV

Conference-Workshop Horizons in Hydrogen Bond Research".

386. B. Reimann, K. Buchhold, H.-D. Barth, B. Brutschy, P. Tarakeshwar, and K. S. Kim, “Anisole-(H2O)n (n=1-3) complexes: An experimental and theoretical investigation of the modulation of optimal structures, binding energies and vibrational spectra in both the ground and first excited states”, J. Chem. Phys. 117,8805-8822 (2002).
387. J. H. Cho, L. Kleinman, K.-J. Jin, and K. S. Kim, “Theoretical study of water adsorption on the Ge(100) surface”, Phys. Rev. B 66, 113306 (2002).
388. H. Ihm, S. Yun, H. G. Kim, J. K. Kim, and K. S. Kim, “Tripodal Nitro-Imidazolium Receptor for Anion Binding Driven by (C-H)+---X- Hydrogen Bonds”, Org. Lett. 4, 2897-2900 (2002).
389. S. Yun, D. S. Jang, G. Choi, K. S. Kim, K. Y. Choi, and H. C. Lee, “Trifluoroethanol increases the Stability of Δ5-3-Ketosteorid isomerase: 15N NMR Relaxation Studies”, J. Biol. Chem. 277, 23414-23419 (2002).
390. H. M. Lee and K. S. Kim, “Structure, electronic properties, and vibrational spectra of the water octamer with an extra electron: Ab Initio Study”, J. Chem. Phys. 117, 706-708 (2002).
391. J. M. Park , P. Tarakeshwar, K.S. Kim, and Tim Clark, “Nature of the interaction of paramagnetic atoms (A=4N, 4P, 3O, 3S) with π systems and C60: A theoretical investigation of A•••C6H6 and endohedral fullerenes A@C60”, J. Chem. Phys. 116, 10684-10691 (2002).
392. S. Hu, J, Kim, P. Tarakeshwar, and K. S. Kim, “Insights into the Nature of SiH4-BH3 Complex: Theoretical Investigation of New Mechanistic Pathways Involving SiH3• and BH4• Radicals”, J. Phys. Chem. A 106, 6817-6822 (2002).
393. K. S. Kim, “Self-assembled organic nanotubes and self-synthesized silver subnanowire arrays in an ambient solution phase”, Curr. Appl. Phys. 2, 65-69 (2002).
394. K. S. Kim, D. Kim, J. Y. Lee, P. Tarakeshwar, and K. S. Oh, “Catalytic Mechanism of Enzymes: Preorganization, Short Strong Hydrogen Bond, and Charge Buffering”, Biochemistry 41, 5300-5306 (2002).
395. H. M. Lee, J. Kim, C.-J. Kim, and K.S. Kim, Ab initio study of the isomerization of retinal chromophore and its derivatives, J. Chem. Phys. 116, 6549-6559 (2002).
396. H. M. Lee and K.S. Kim, "Ab Initio Study of Superoxide Anion-Water Clusters O2-(H2O)n=1-5", Mol. Phys. 100, 875-879 (2002).
397. H. S. Choi, D. Kim, P. Tarakeshwar, S.B. Suh, and K.S. Kim, "A New Type of Ionophore Family utilizing the Cation-Olefinic pi Interaction: Theoretical Study of [n] Beltenes", J. Org. Chem. 67, 1848-1851 (2002).
398. H. M. Lee, D. Kim, and K.S. Kim, "Structures, spectra, and electronic properties of halide-water pentamers and hexamer, X-(H2O)5,6 (X=F, Cl, Br, I): Ab initio study", J. Chem. Phys. 116, 5509-5520 (2002)
399. J. H. Cho, D.-W. Oh, K.S. Kim, and L. Kleinman, "Adsorption structure of 1,4-cyclohexadiene on Si(001)", J. Chem. Phys. 116, 3800-3804 (2002).
400. S. J. Youn, B.R. Sahu, and K.S. Kim, "Large orbital magnetic moment and coulomb correlation effects in FeBr2", Phys. Rev. B. 65, 052415 (2002).
401. S. B. Suh, C. Cui, H.S. Son, J.S. U, Y. Won, and K.S. Kim, "Novel amphi-ionophore in aqueous solution: cyclohexaalaryl", J. Phys. Chem. B 106, 2061-2064 (2002).
402. J. Y. Lee, K. S. Kim, B. J. Mhin, "Intramolecular charge transfer of pi-conjugated push--pull systems in terms of polarizability and electronegativity", J. Chem. Phys. 115, 9484-9489 (2001).
403. B.H. Hong , S.C. Bae, C.-W. Lee, S. Jeong, and K.S. Kim, Ultrathin Single-crystalline Silver Nanowire Arrays Formed in an Ambient Solution Phase, **Science** 294, 348-351 (2001); published online September 6, 2001 (10.1126/science.1062126). *Highlighted in C&EN.*
404. J.-H. Cho, D.-H. Oh, K.S. Kim, L. Kleinman, "Weakly correlated one-dimensional indium chains on Si(111)", Phys. Rev. B. 64 235302 (2001).
405. C.Riehn, B. Reimann, K. Buchhold, H.-D. Barth, S. Vaupel, B. Brutschy, P.Tarakeshwar, and K. S. Kim, "On the microscopic interaction of p-chlorofluorobenzene with water", J. Chem. Phys. 115, 10045-10047 (2001).

406. B. H. Hong, J. Y. Lee, C.-W. Lee, J. C. Kim, S. C. Bae, and K. S. Kim, “Self-Assembled Arrays of Organic Nanotubes with Infinitely Long One-Dimensional H-Bond chains”, J. Am. Chem. Soc. 123(43), 10748-10749 (2001). *Highlighted in C&EN.*
407. K.S. Oh, J. Yoon, K.S. Kim, "Structural Stabilities and Self-Assembly of Cucurbit[n]uril (n=4-7) and Decamethylcucurbit[n]uril(n=4-6):A Theoretical Study", J. Phys. Chem. B 105, 9726-9731 (2001).
408. P. Tarakeshwar and K.S. Kim, E. Kraka and D. Cremer, "Structure and stability of fluorine-substituted benzene-argon complexes: The decisive role of exchange-repulsion and dispersion interactions", J. Chem. Phys. 115, 6018-6029 (2001).
409. S.J. Chung, S. Chung, H.S. Lee, E.-J. Kim, K.S. Oh, H.S. Choi, K.S. Kim, Y.J. Kim, J.H. Hahn, and D.H. Kim, "Mechanistic Insight into the Inactivation of Carboxypeptidase A by Benzyl-2-oxo-1,3-oxazolidine-4-acetic Acid, a Novel Type of Irreversible Inhibitor for Carboxypeptidase A with No Stereospecificity”, J. Org. Chem. 66, 6462-6471 (2001).
410. I. Park, K. Cho, S. Lee, K.S. Kim and J.D. Joannopoulos, “Ab initio atomistic dynamical study of an excess electron in water”, Computational Materials Science. 21, 291-300(2001).
411. H.M. Lee, S.B. Suh, and K.S. Kim, "Structures, energies, and vibrational spectra of water undecamer and dodecamer: An ab initio study", J. Chem. Phys. 114, 10749-10756 (2001). Error: 115, 7331 (2001).
412. J.-H. Cho, L. Kleinman, C.T. Chan, K.S. Kim, "First-principles study of the adsorption of C2H2 and C2H4 on Si(100)", Phys. Rev. B 63, 073306 (2001).
413. J.-H. Cho and K.S. Kim, C.T. Chan, Z. Zhang, "Oscillatory energetics of flat Ag films on MgO(001)", Phys. Rev. B 63, 113408 (2001).
414. Zhao H. K.S. Kim, "Model calculation of the band energy gap for poly(p-phenylenevinylene), J. Phys.-Cond. Mat.13, 579-593 (2001).
415. P. Tarakeshwar, H. S. Choi, and K. S. Kim, "Olefinic vs. aromatic pi-H interaction: A theoretical investigation of the nature of interaction of first-row hydrides with ethene and benzene", J. Am. Chem. Soc. 123, 3323-3331 (2001).
416. H.M. Lee and K.S. Kim, "Structures and spectra of iodide-water clusters I-(H2O)n=1-6: An ab initio study", J. Chem. Phys. 114, 4461-4471 (2001).
417. P. Tarakeshwar, H.S. Choi, and K.S Kim, S. Djafari, K. Buchhold, B. Reimann, H.-D. Barth and B. Brutschy, "Ab initio studies of pi-water tetramer complexes. Evolution of optimal structures, binding energies and vibrational spectra of pi-(H2O)n(n=1-4) complexes", J. Chem. Phys.114, 4016-4024 (2001).
418. H.S. Son, B.H. Hong, C.-W. Lee, S. Yun, K.S. Kim, "A New Type of Helix Pattern in Poly-Alanine Peptide", J. Am. Chem. Soc. 123, 514-515 (2001). *Highlighted in C&EN.*
419. P. Tarakeshwar, K.S. Kim, B. Brutschy, " to conformational transition: Interactions of the water trimer with p-systems", J. Chem. Phys. 114, 1295-1305 (2001).
420. H. S. Choi and K.S. Kim, "Theoretical Study of Microscopic Molecular Structure of Helicenebisquinone Aggregates", J. Phys. Chem. B. 104, 11006-11009 (2000).
421. C. Riehn, A. Degen, A.Weichert, M.Bolte, E.Egert, B.Brutschy, P.Tarakeshwar and K.S.Kim, "The molecular structure of para-cyclohexylaniline. Comparison of results obtained by X-ray diffraction with gas phase laser experiments and ab initio calculations", J. Phys. Chem. A 104, 11593-11600 (2000).
422. K. S. Oh, S.-S. Cha, D.-H. Kim, H.-S. Cho, N.-C. Ha, G. Choi, J. Y. Lee, P. Tarakeshwar, H. S. Son, K. Y. Choi, B.-H. Oh, and K. S. Kim, "Role of Catalytic Residues in Enzymatic Mechanisms of Homologous Ketosteroid Isomerases", Biochemistry 39, 13891-13896 (2000).
423. K. S. Kim, P. Tarakeshwar, J. Y. Lee, "Molecular Clusters of π-Systems: Theoretical Studies of Structures, Spectra and Origin of Interaction Energies", **Chem. Rev.** 100, 4145-4185 (2000).
424. C.-W. Lee, E.J. Jung, S.J. Lee, K.H. Ahn, K.S. Kim, "Synthesis of Unsymmetrical Chiral Triaza-18-crown-6 and Diaza-12-crown-4 with a Pendant Group", J. Org. Chem. 65, 7225-7227 (2000).
425. J.Y. Lee, J. Kim, H.M. Lee, P. Tarakeshwar, and K.S. Kim, "Structures, vibrational frequencies, and IR spectra of the hexa-hydrated benzene clusters", J. Chem. Phys. 113, 6160-6168 (2000).
426. J. Kim, H.M. Lee, S.B. Suh, D. Majumdar, and K.S. Kim, "Comparative ab initio study of the

structures, energetics and spectra of X-(H2O)n=1-4[X=F, Cl, Br, I] clusters", J. Chem. Phys. 113, 5259-5272 (2000).

427. S.B. Suh, H.M. Lee, J. Kim, J.Y. Lee, and K.S. Kim, "Vibrational spectra and electron detachment energy of the anionic water hexamer", J. Chem. Phys. 113, 5273-5277 (2000).
428. K. S. Oh, C.-W. Lee, H.S. Choi, S.J. Lee, K.S. Kim, "Origin of the High Affinity and Selectivity of Novel Receptors for NH4+ over K+: Charged Hydrogen Bonds vs. Cation-pi Interaction", Org. Lett. 2, 2679-2681(2000).
429. J.-H. Cho, J.M. Park, and K.S. Kim, "Influence of intermolecular hydrogen bonding on water dissociation at the MgO(001) surface", Phys. Rev. B. 62, 9981-9984 (2000).
430. D.-H. Oh, J.M. Park, K.S. Kim, "Structures and electronic properties of small carbon nanotube tori", Phys. Rev. B. 62, 1600-1603 (2000).
431. H.M. Lee, S.B. Suh, and K.S. Kim, "Structure of the Water Hexamer Anion", Bull. Korean. Chem. Soc. 21, 555-556 (2000).
432. C.-W. Lee, K. S. Oh, K. S. Kim, and K. H. Ahn, "Suppressed **β**-Hydride Elimination in Palladium-Catalyzed Cascade Cyclization-Coupling Reactions: An Efficient Synthesis of 3-Arylmethylpyrrolidines", Org. Lett. 2, 1213-1216 (2000).
433. J.-H. Cho and K. S.Kim, "Hydrogen-bonded array of NH2 on the Si(100) surface", Phys. Rev. B. 62, 1607-1610 (2000).
434. K. S. Kim, K. S. Oh, and J. Y. Lee, "Catalytic role of enzymes: Short strong H-bond induced partial proton shuttles and charge redistributions", Proc. Natl. Acad. Sci. USA 97, 6373-6378 (2000).
435. H. M. Lee, S. B. Suh, J. Y. Lee, P. Tarakeshwar, and K. S. Kim, "Structures, energies, vibrational spectra, and electronic properties of water monomer to decamer", J. Chem. Phys. 112, 9759-9772 (2000). Error: 114, 3343 (2001).
436. J. Yoon, K. S. Kim, and K. K. Baeck, "Ab initio study of the low-lying electronic states of Ag3- Ag3, and Ag3+: A coupled-cluster approach", J. Chem. Phys. 112, 9335-9342 (2000).
437. B. J. Mhin and W. Y. Chang, J. Y. Lee, K.S. Kim, "Ab initio study of peroxyacetic nitric anhydride and peroxyacetryl radical: Characteristic infrared band of peroxyacetyl radical", J. Phys. Chem. A. 104, 2613-2617 (2000).
438. K. S. Kim, J. M. Park, J. Kim, S. B. Suh, and P. Tarakeshwar, K. H. Lee, S. S. Park, "Dimer to Monomer Phase Transition in Alkali-metal Fullerides: Magnetic Susceptibility Changes", Phys. Rev. Lett. 84, 2425-2428 (2000).
439. J.-H. Cho, K.S. Kim, S. H. Lee, M. H. Kang, and Z. Y. Zhang, "Origin of contrasting surface core-level shifts at the Be(1010) at the MgO(100) surfaces", Phys. Rev. B. 61, 9975-9978 (2000).
440. J.-H. Cho, K.S. Kim, S.-H. Lee, M.-H. Kang, "Dissociative adsorption of water on the Si(001) surface: A first-principles study", Phys. Rev. B. 61, 4503-4506 (2000).
441. A. V. Plyukhin and K. S. Kim, "Discrete velocity random motion in an external field", Phys. Rev. E. 61, 3207-3211 (2000).
442. K. Buchhold, B. Reimann, S. Djafari, H.-D. Barth, and B. Bruthschy, P. Tarakeshwar and K. S. Kim, "Fluorobenzene and p-difluorobenzene microsolvated by methanol: An infrared spectroscopic and ab initio theoretical investigation", J. Chem. Phys. 112, 1844-1858 (2000).
443. P. Tarakeshwar, K. S. Kim, B. Brutschy, "Interaction of the water dimer with pi-systems: A theoretical investigation of structures, energies, and vibrational frequencies", J. Chem. Phys. 112, 1769-1781 (2000).
444. C. Riehn, K. Buchhold, B. Reimann, S. Djafari, H.-D. Brath, and B. Brutschy, P. Tarakeshwar and K. S. Kim, "van der Waals isomers and ionic reactivity of the cluster system para-chlorofluorobenzene/methanol", J. Chem. Phys. 112, 1170-1177 (2000).
445. D. Majumdar, G.-S. Kim, J. Kim, K. S. Oh, J. Y. Lee, and K. S. Kim, W.Y. Choi, S.-H. Lee, and M.-H. Kang, B. J. Mhin, "Ab initio investigations on the HOSO2+O2->SO3+HO2 reaction", J. Chem. Phys. 112, 723-730 (2000).
446. J. Y. Lee, S. B. Suh, and K. S. Kim, "Polyenes vs polyyens: Efficient pi-frame for nonlinear optical pathways", J. Chem. Phys. 112, 344-348 (2000).

447. D. Majumdar, J. Kim, and K. S. Kim, "Charge transfer to solvent(CTTS) energies of small X-(H2O)n=1-4 (X=F, CI, Br, I) clusters: Ab initio study, J. Chem. Phys. 112, 101-105 (2000).
448. P. Tarakeshwar and K.S. Kim, "A Theoretical Investigation of Benzene-AlX3 and Ethene-AlX3 (X = H, F, Cl) Interactions", J. Phys. Chem. A. 103, 9116-9124 (1999); Correction 103, 11486 (1999).
449. H.-S. Cho, N.-C. Ha, G. Choi, H.-J. Kim, D. Lee, K.S . Oh, K.S. Kim, W. Lee, K.Y. Choi, B.-H. Oh, "Crystal Structure of 5-3-Ketosteroid Isomerase from Pseudomonas testosteroni in Complex with Equilenin Settles the Correct Hydrogen Bonding Scheme for Transition State Stabilization", J. Biol. Chem. 274(46), 32863-32868 (1999).
450. J. Kim and K. S. Kim, "Water dimer to pentamer with an excess electron: Ab initio study", J. Chem. Phys. 111(22), 10077-10087 (1999).
451. D. Majumdar, H. M. Lee, J. Kim, and K. S. Kim, "Photoswitch and nonlinear optical switch: Theoretical studies on 1,2-bis-(3-thienyl) - ethene derivatives", J.Chem.Phys.111(13), 5866-5872 (1999).
452. P. Tarakeshwar, H. S. Choi, S. J. Lee, J. Y. Lee, K. S. Kim, T.-K. Ha, J. H. Jang, J. G.Lee, and H. Lee, "A theoretical investigation of the nature of the pi-H interaction in Ethene -H2O, Benzene-H2O, and Benzene-(H2O)2 ", J. Chem. Phys.111, 5838-5850 (1999).
453. H. S. Choi, K.S. Kim, "Structures, Magnetic Properties, and Aromaticity of Cyclacenes", Angew. Chem. Int. Ed. 38(15) 2256-2258 (1999); Angew. Chem. 111, 2400-2402 (1999).
454. H.M. Lee, J. Kim, S. Lee, B.J. Mhin, and K.S. Kim, "Aqua-potassium (I) complexes: Ab initio study", J. Chem. Phys. 111, 3995-4004 (1999).
455. B. H. Hong, J. Y. Lee, S. J. Cho, S. Yun, and K. S. Kim, "Theoretical Study of the Conformations and Strain Energies of [n,n]metaparacyclophanes: Indication of Stable Edge-to-face and Displaced Face-to-face Conformers for n=4", J. Org. Chem. 64, 5661-5665 (1999).
456. P. Tarakeshwar, K.S. Kim, and B. Brutschy, "Fluorobenzene...water and difluorobenzene...water systems: An ab initio investigation", J. Chem. Phys. 110, 8501-8512 (1999).
457. J. Baik, J. Kim, D. Majumdar, and K.S. Kim, "Structures, energetics, and spectra of fluoride-water clusters F-H2O)n, n=1-6: Ab initio study", J. Chem. Phys. 110, 9116-9127 (1999).
458. J. Kim, D. Majumdar, H.M. Lee, and K.S. Kim, "Structures and energetics of the water heptamer: Comparison with the water hexamer and octamer", J. Chem. Phys. 110, 9128-9134 (1999).
459. H. S. Park, K. S. Oh, K. S. Kim, T. Chang, D. R. Spiegel, "Change of Internal Hydrogen Bonding of Methyl Red upon Photoisomerization Monitored by Forced Rayleigh Scattering", J. Phys. Chem. B 103, 2355-2360 (1999).
460. C. Cui and K.S. Kim, "Cation Affinities of Cyclohexadepsipeptide: Ab Initio Study", J. Phys. Chem. A 103, 2751-2755 (1999).
461. J. Kim, J.Y. Lee, K.S. Oh, J.M. Park, S. Lee, and K.S. Kim, "Quantum-mechanical probabilistic structure of the water dimer with an excess electron", Phys. Rev. A. 59, R930-933(1999).
462. P. Tarakeshwar, S.J. Lee, J.Y. Lee, and K. S. Kim, "An ab initio study of benzene-BX3 (X=H,F,Cl) Interactions", J. Phys. Chem. B 103, 184-191 (1999).
463. J. Kim, K. S. Kim, "Structures, binding energies, and spectra of isoenergetic water hexamer clusters: Extensive ab initio studies", J. Chem. Phys. 109, 5886-5895 (1998).
464. H.S. Choi,S.B. Suh, S.J. Cho, and K.S. Kim, "Ionophores and receptors using cation-π interactions: Collarenes", Proc. Natl. Acad. Sci. USA 95, 12094-12099 (1998).
465. P. Tarakeshwar, S.J. Lee, J.Y. Lee, and K. S. Kim, "Benzene-hydrogen halide interactions: Theoretical studies of binding energies, vibrational frequencies, and equilibrium structures", J. Chem. Phys. 108, 7217-7223 (1998).
466. P. Tarakeshwar, J.Y. Lee, and K.S. Kim, "Role of Lewis Acid(AlCl3)-Aromatic Ring Interactions in Friedel-Craft's Reaction: An ab Initio Study", J. Phys. Chem. A.102, 2253-2255 (1998).
467. C. Cui, S.J. Cho, K.S. Kim, "Cation Affinities of [16]Starand Model- Comparison with 12-Crown-4: Crucial Role of Dipolar Moiety Orientations", J. Phys. Chem. A. 102, 1119-1123 (1998).
468. K.S. Kim, C. Cui, S.J. Cho, "Novel Amphi-ionophores", J. Phys. Chem. B. 102, 461-463 (1998).
469. C. Cui, S.J. Cho, K.S. Kim, C. Baehr, and J.C. Jung, "Rotational conformational energetics of stiff

aromatic polyimides: effects of exchange repulsions, dipole-moiety interactions, and pi-conjugations", J. Chem. Phys. 107, 10201-10206 (1997). doi: 10.1063/1.474156

470. T. Ren, Y. H. Yin, K.S. Kim, and D.H. Kim, "Aromatic-Aromatic Ring Interaction Revisited with Model Compounds of Wilcox", J. Biomol. Struct. Dynamics 15, 401-405 (1997).
471. S. Lee, J. Kim, S.J. Lee, and K.S. Kim, "Novel Structures for the Excess Electron state of the Water Hexamer and the Interaction Forces Governing the Structures", Phys. Rev. Lett. 79, 2038-2041 (1997).
472. K.S. Kim, S. Lee, J. Kim, and J.Y. Lee, "Molecular Cluster Bowl to Enclose a Single Electron", J. Am. Chem. Soc. Comm. 119, 9329-9330 (1997).
473. J.Y. Lee and K.S. Kim, "Relationship between spectral intensities and nonlinear optical properties", J. Chem. Phys. 107, 6515-6520 (1997).
474. J.Y. Lee, B.J. Mhin, and K.S. Kim, "Roles of central and terminal carbon atoms in infrared and Raman intensities of polyenes: Analysis of atomic polar and polarizability tensors derivatives", J. Chem. Phys. 107, 4881-4885 (1997).
475. J.Y. Lee, S.J. Lee, and K.S. Kim, "Raman intensities of C=C stretching vibrational frequencies of polyenes: Nodal mode analysis", J. Chem. Phys. 107, 4112-4117 (1997).
476. J. Kim, J.M. Park, K.S. Oh, J.Y. Lee, S. Lee, and K. S. Kim, "Structure and vertical electron-detachment energy, and O-H stretching frequencies of e+(H2O)12", J. Chem. Phys. 106, 10207-10214 (1997).
477. S.J. Cho, C. Cui, J.Y. Lee, J.K. Park, S.B. Suh, J. Park, B.H. Kim, and K.S. Kim, "N-Protonation vs. O-protonation in Strained Amides: Ab initio Study", J. Org. Chem. 62, 4068-4071 (1997).
478. K.S. Kim, S.J. Cho, K.S. Oh, J.S. Son, J. Kim, J.Y. Lee, S. Lee, S.J. Lee, Y.-T.Chang, S.-K. Chung, T.K. Ha, B.S. Lee, and I. Lee, "Theoretical Studies of Regioselectivity of Myo-Inositol Derivatives: Importance of Solvent Dielectric Constants", J. Phys. Chem. A 101, 3776-3783 (1997).
479. K.S. Kim, J.Y. Lee, H.S. Choi, J. Kim, and J.H. Jang, "Quantum mechanical probabilistic structure of the benzene-water complex", Chem. Phys. Lett. 265, 497-502 (1997).
480. S. Lee, J. Kim, J.K. Park , and K.S. Kim, "Ab Initio Study of the Structures, Energetics and Spectra of Aqua-Zinc(II)", J. Phys. Chem. 100, 14329-14338 (1996).
481. S.J. Lee, S.J. Cho, K.S. Oh, C. Cui, Y. Ryu, Y.-T. Chang, K.S. Kim, and S.-K. Chung, "Ab Initio Conformational Study of 1,2:4,5-Di-o-isopropylidene-myo-Inositol", J. Phys. Chem. 100, 10111-10115 (1996).
482. S. Lee, S.J. Lee, J.Y. Lee, J. Kim, K.S. Kim, I. Park, K. Cho, and J.D. Joannopoulos, "Ab Initio Study of Water Hexamer Anions", Chem. Phys. Lett. 254, 128-134 (1996).
483. K.S. Kim, I. Park, S. Lee, K. Cho, J.Y. Lee, J. Kim, and J.D. Joannopoulos, "The Nature of a Wet Electron", Phys. Rev. Lett. 76, 956-959 (1996).
484. S.J. Cho, H. Hwang, J.M. Park , K.S. Oh, K.S. Kim, "Starands vs. Ketonands: Ab Initio Study", J. Am. Chem. Soc. 118, 485-486 (1996).
485. J.K. Park , S.J. Cho, S. Lee, K. S. Kim, and D.H. Kim, "Conformational Energies of Substrates and Inhibitors for Carboxypeptidase A: Stereoelectronic Effect", J. Biomol. Struct. Dynamics 12, 1033-1040 (1995).
486. J.Y. Lee, O. Hahn, S.J. Lee, H. S. Choi, B.J. Mhin, M.S. Lee, and K.S. Kim, "Vibrational Spectra of all-trans-1,3,5,7-Octatetraene", J. Phys. Chem. 99, 2262-2266 (1995).
487. J.Y. Lee, O. Hahn, S.J. Lee, H. S. Choi, H. Shim, B.J. Mhin, and K.S. Kim, "Ab Initio Study of s-trans-1,3-Butadiene using Various Levels of Basis Set and Electron Correlation: Force Constants and Exponentially Scaled Vibrational Frequencies", J. Phys. Chem. 99, 1913-1918 (1995).
488. J.Y. Lee, S.J. Lee, H. S. Choi, S.J. Cho, K.S. Kim, and T.K. Ha, "Ab Initio Study of the Complexation of Benzene with Ammonium Cations", Chem. Phys. Lett. 232, 67-71 (1995).
489. J. Kim, S. Lee, S.J. Cho, B.J. Mhin, and K.S. Kim, "Structures, Energetics, and Spectra of aqua-sodium(I): Thermodynamic Effects and Nonaddtive Interactions", J. Chem. Phys. 102, 839-849 (1995).
490. J. Kim, J.Y. Lee, S. Lee, B.J. Mhin, and K.S. Kim, "Harmonic Vibrational Frequencies of the Water Monomer and Dimer: Comparison of Various Levels of Ab Initio Theory", J. Chem. Phys. 102, 310-317 (1995).

491. D.H. Kim, K.S. Kim, and J.K. Park, "A Three-Dimensional Active Site Model of Carboxypeptidase A", Bull. Korean Chem. Soc. 15, 805-807 (1994).
492. S. Lee, S.J. Cho, J.K. Park , H.-S. Kim, and K.S. Kim, "Comparable Structural Stabilities of Penta- and Hexa-coordinate Zn(II) in a Simple Model System of the Active Site of Carboxypeptidase A", Bull. Korean Chem. Soc. 15, 774-776 (1994).
493. K.S. Kim, J.Y. Lee, S.J. Lee, T.-K. Ha, and D.H. Kim, "On Binding Forces between Acc. Ring and Quaternary Ammonium Compound", J. Am. Chem. Soc. 116, 7399-7400 (1994).
494. J. Kim, B.J. Mhin, S.J. Lee, and K.S. Kim, "Entropy-driven Structures of the Water Octamer", Chem. Phys. Lett. 219, 243-246 (1994).
495. B.J. Mhin, J. Kim, S. Lee, J.Y. Lee, and K.S. Kim, "What is the Global Minimum Energy Structure of the Water Hexamer? Importance of Nonadditive interactions", J. Chem. Phys. 100, 4484-4486 (1994).
496. S.J. Lee, B.J. Mhin, S.J. Cho, J.Y. Lee, and K.S. Kim, "Ab Initio Studies of the Conformations of Methylamine and Ethylenediamine: Interaction Forces Affecting the Structural Stability", J. Phys. Chem. 98, 1129-1134 (1994).
497. K.S. Kim, S. Lee, B.J. Mhin, S.J. Cho, and J. Kim, "Structures and Energetics of Zn(NH3)n2+ (n=4-6): Coordination Number of Zn2+ by Ammine", Chem. Phys. Lett. 216, 309-312 (1993).
498. B.J. Mhin, J. Kim, and K.S. Kim, "Entropy-driven Structures of the Hexa-Aqua-Sodium(I)", Chem. Phy. Lett. 216, 305-308 (1993).
499. B.J. Mhin, S.J. Lee, and K.S. Kim, "Water Cluster Distribution with respect to Pressure and Temperature in the Gas Phase", Phys. Rev. A 48, 3764-3770 (1993).
500. K.S. Kim, B.H. Kim, W.M. Park, S.J. Cho, and B.J. Mhin, "Origin of Diastereoselectivity in the Nitrile Oxide Cycloadditions with Oppolzer's Chiral Sultams: Coulombic Interaction as the Key Role in Diastereofacial Differentiation", J. Am. Chem. Soc. 115, 7472-7477 (1993).
501. K.S. Kim, "Macromolecular Modeling and NMR Distance Geometry Refinement", Bull. Korean Chem. Soc. 14, 18-20 (1993).
502. U-S. Choi and K.S. Kim, "Theoretical Study of the Nonlinear Optical Properties of Nonsubstituted-, Methylfluoro-, and Amino-nitro-Polyenes", Bull. Korean Chem. Soc. 14, 14-16 (1993).
503. S. Kim, C.W. Yoon, B.J. Mhin, H.S. Kim, and K.S. Kim, "Photorealistic Image Generation of Molecular Structure on PC Screen Using the Ray-tracing Technique", J. Mol. Graphics, 10, 218-221 (1992).
504. K.S. Kim, B.J. Mhin, U-S. Choi, and K. Lee, "Ab Initio Studies of the Water Dimer Using Large Basis Sets: The Structure and Thermodynamic Energies", J. Chem. Phys. 97, 6649-6662 (1992).
505. Y. Xie, H.F. Schaefer, J.W. Jang, B.J. Mhin, H.S. Kim, C.W. Yoon, and K.S. Kim, "Sulfur Clusters: Structure, Infrared, and Raman Spectra of Cyclo-S6 and Comparison with the Hypothetical Cyclo-O6 Molecule", Mol. Phys. 76, 537-546 (1992).
506. B.J. Mhin, S. Lee, S.J. Cho, K. Lee, and K.S. Kim, "Zn(H2O)6(II) is very Stable among Aqua-Zn(II) Ions", Chem. Phys. Lett. 197, 77-80 (1992).
507. H.S. Kim, B.J. Mhin, C.W. Yoon, C.X. Wang, and K.S. Kim, "A Theoretical Study of a Z-DNA Crystal : Structure of Counterions, Water, and DNA Molecules", Bull. Korean Chem. Soc. 12, 214-220 (1991).
508. B.-J. Mhin, H.S. Kim, H.S. Kim, J.W. Yoon, and K.S. Kim, "Ab Initio Studies of the Water Hexamer: Near Degenerate Structures", Chem. Phys. Lett. 176, 41-45 (1991).
509. C. Liang, Y. Xie, H.F. Schaefer, K.S. Kim, and H.S. Kim, "The Vibrational Spectra of Butatriene (C4H4) and Pentatetraene (C5H4): Is Pentatetraene Bent?", J. Am. Chem. Soc. 113, 2452-2459 (1991).
510. K.S. Kim, H.S. Kim, J.H. Jang, H.S. Kim, B.-J. Mhin, Y.Xie, and H.F.Schaefer, "Hydrogen Bonding Between the Water Molecule and the Hydroxyl Radical (H2O.OH): The 2A" and 2A' Minima", J. Chem. Phys. 94, 2057-2062 (1991).
511. K.S. Kim, J.H. Jang, S. Kim, B.-J. Mhin, and H.F. Schaefer, "Potential New High Energy Density Materials: Cyclooctaoxygen O8, Including Comparisons with the Well-known Cyclo-S8 Molecule", J. Chem. Phys. 92, 1887-1892 (1990).
512. K.S. Kim, H.S. Kim, S. Kim, J.H. Jang, and H.F. Schaefer, "Cyclododecaoxygen, O12: Comparison

with the Experimentally Characterized S12 Molecule", J. Am. Chem. Soc. 111, 7746-7749 (1989).

513. K.S. Kim, "On Effective Methods to Treat Solvent Effects in Macromolecular Mechanics and Simulations", Chem. Phys. Lett. 159, 261-267 (1989).
514. K.S. Kim and E. Clementi, "Hydration Structures and Energetics of Phospholipid", J. Comput. Chem. 8, 57-66 (1987).
515. K.S. Kim, D.P. Vercauteren, M. Welti, S.L. Fornili, and E. Clementi, "Interactions of Na+ Ion with the Solvated Gramicidin A Transmembrane Channel", Croat. Chem. Acta, 59, 369-381 (1986).
516. K.S. Kim, M. Dupuis, G.C. Lie, and E. Clementi, "Revisiting small clusters of water molecules", Chem. Phys. Lett. 131, 451-456 (1986).
517. K.S. Kim and E. Clementi, "Hydration Analysis of the Intercalated Complex of Deoxydinucleoside Phosphate and Proflavine: Computer Simulations", J. Phys. Chem. 89, 3655-3663 (1985).
518. K.S. Kim, H.L. Nguyen, P.K. Swaminathan, and E. Clementi, "Na+ and K+ Ion Transport in a Solvated Gramicidin A Transmembrane Channel: Molecular Dynamics Studies Using Parallel Processors", J. Phys. Chem. 89, 2870-2876 (1985).
519. K.S. Kim, "Microscopic Effect of an Applied Voltage on the Solvated Gramicidin A Transmembrane Channel in the Presence of Na+ and K+ Cations", J. Comput. Chem. 6, 256-263 (1985).
520. K.S. Kim and E. Clementi, "Energetics and Hydration Structures of a Solvated Gramicidin A Transmembrane Channel for K+ and Na+ Cations", J. Am. Chem. Soc. 107, 5504-5513 (1985).
521. K.S. Kim and E. Clementi, "Energetics and Pattern Analysis of Crystals of Proflavine Deoxydinucleoside Phosphate Complex", J. Am. Chem. Soc. 107, 227-234 (1985).
522. K.S. Kim, D.P. Vercauteren, M. Welti, S. Chin, and E. Clementi, "Interactions of K+ Ion with the Solvated Gramicidin A Transmembrane Channel", Biophys. J. 47, 327-335 (1985).
523. M.R. Hoffmann, W.D. Laidig, K.S. Kim, D.J. Fox, and H.F. Schaefer, "Electronic Symmetry Breaking in Polyatomic Molecules. Multi Configuration Self-consistent Field Study of the Cyclopropenyl Radical C3H3", J. Chem. Phys. 80, 338-343 (1984).
524. K.S. Kim, G. Corongiu, and E. Clementi, "Networks of Water Molecules in a Proflavine Deoxydinucleoside Phosphate Complex", J. Biomol. Struct. Dynamics 1, 263-285 (1983).
525. K.S. Kim, H.F. Schaefer, L. Radom, J.A. Pople, and J.S. Binkley, "Vibrational Frequencies of the HCCN Molecule. A Near Degeneracy Between Bent Cyanocarbene and Linear Allene-Related Geometries", J. Am. Chem. Soc. 105, 4148-4154 (1983).
526. K.S. Kim, S.P. So, and H.F. Schaefer, "Structure and Energetics of Realistic Carbynes: Carbohydroxycarbyne, (HOCOC:.)", J. Am. Chem. Soc. 104, 1457-1461 (1982).
527. Y. Osamura, J.D. Goddard, H.F. Schaefer, and K.S. Kim, "Near Degenerate Rearrangement between the Radical Cations of Formaldehyde and Hydroxymethylene", J. Chem. Phys. 74, 617-621 (1981).
528. K.S. Kim and H.F. Schaefer, "Geometrical Isomerism in Triplet Carbenes: Carbohydroxycarbene", J. Am. Chem. Soc. 102, 5389-5390 (1980).

Books/Monographs

1. C. E. Dykstra, G. Frenking, K. S. Kim, and G. E. Scuseria (editors), “Theory and Applications of Computational Chemistry: The First 40 Years”, Elsevier) 2005 (pp. 1-1308).

(Book-Chapters)

2. K. C. Kemp, Y. Cho, V. Chandra, K. S. Kim, Noncovalenet functionalization of graphene, in “Functionalisation of graphene”, edited by V. Georgakilas, Wiley, 2014. Pp. 199-217.
3. Y. Cho, S. K. Min, J. Y. Lee, W. Y. Kim, Kwang S. Kim, Computer Aided Nanomaterials Design – Selfassembly, Nanooptics, Molecular electronics/spintronics, and Fast DNA sequencing, in “Practical Aspects of Computational Chemistry I: An Overview of the Last Two Decades and Current Trends”, edited by J. Leszczynski, M. K. Shukla, and H. de Rode, Springer, 2012, pp. 319-346.

4. W. Y. Kim and K. S. Kim, Molecular spintronics, in “Computational Methods for Large Systems: Electronic Structure Approaches for Biotechnology and Nanotechnology”, edited by J. R. Reimers, John Wiley & Sons, Inc. Hoboken, NJ, 2011, pp. 589-614.
5. M. Kołaski, A. Kumar, H. M. Lee, and K. S. Kim, Charge transfer in excited states: Ab initio molecular dynamics simulations, in **“**Hydrogen Bonding in Excited States". Edited by K.-L. Han and G.-J. Zhao, John Wiley & Sons, 2010, pp. 627-640.
6. H. M. Lee, N. J. Singh, and K. S. Kim. Weak to strong hydrogen bonds, in “Hydrogen Bonding-New Insights”, edited by S. J. Grabowski. Springer, Dontrecht, Netherlands, 2006, pp 149-192.
7. K. S. Kim, P. Tarakeshwar, and H. M. Lee, Clusters to functional Molecules, Nanomaterials, and Molecular Devices: Theoretical Exploration, in “Theory and Applications of Computational Chemistry: The First 40 Years”, Edited by C. E. Dykstra, G. Frenking, K. S. Kim, and G. E. Scuseria, Elsevier, 2005, pp. 963-993.
8. C. E. Dykstra, G. Frenking, K. S. Kim, P. and G. E. Scuseria, “Computing technologies, theories, and algorithms. The making of 40 years and more of theoretical and computational chemistry”, in “Theory and Applications of Computational Chemistry: The First 40 Years”, Edited by C. E. Dykstra, G. Frenking, K. S. Kim, and G. E. Scuseria, Elsevier, 2005, pp. 1-7.
9. K. S. Kim, P. Tarakeshwar, and H. M. Lee, De novo theoretical design of functional nanomaterials and molecular devices, In "Dekker Encyclopedia of Nanoscience and Nanotechnology", Edited by J. A. Schwarz, C. Contescu, and K. Putyera, Marcel Dekker Inc., New York, 2004, Vol. 3, pp.2423-2433.
10. P. Tarakeshwar, D. Kim, H. M. Lee, S. B. Suh and K. S. Kim, Theoretical Approaches to the Design of Functional Nanomaterials, In ""Computational Material Science, (Theoretical and Computational Chemistry), Edited by J. Leszczynski, Elsevier Publishers, Amsterdam, 2004, Vol. 15, pp.119-170.
11. P. Tarakeshwar and K.S. Kim, Nanorecognition, In "Encyclopedia of Nanoscience and Nanotechnology", Edited by H. S. Nalwa, American Science Publishers, California, 2004., Vol. 7, pp.367-404.
12. P. Tarakeshwar, H. M. Lee, and K.S. Kim, Insights from theoretical investigations of aqueous clusters, In "Reviews in Modern Quantum Chemistry - A celebration of the contributions of R.G. Parr", Edited by K.D. Sen, World Scientific, Singapore, 2002, pp. 1642-1683.
13. K.S. Kim, Ion transport in the Gramicidin A transmembrane channel: Monte Carlo and Molecular Dynamics simulations, Physics of Complex Fluids and Biological Systems, Edited by W. Sung, Y.H. Jeong, and S.I. Choi, Min Eum Sa, Seoul . Korea, 1993.
14. R.M. Levy, F. Hirata, K.S. Kim, and P. Zhang, "Probing the Structure and Dynamics of Biopolymers with Computer Simulations", Am. Chem. Soc. Symposium Series, 353, 82-105 (1987).

Patents :

1. B. H. Hong, J. Y. Lee, and K.S. Kim, “Synthesis and applications of nanoscale lens through self-assembly process”, Patent No: 10-1166415, Registration Date : 2012.07.11, Application No:10-2009-0084121 (2009.9.7), Country Registered: Korea
2. S. K. Min, W. Y. Kim, Y. Cho, K. S. Kim, “Device and method for ultrafast DNA sequencing based on graphene nanoribbons”, Patent No: 10-12972226, Registration Date : 2013.8.9, Application No: 10-2011-0056530 (2011.06.10), Country Registered: Korea [그래핀 나노리본을 이용한 초고속 염기서열 분석 소자 및 방법]
3. B. H. Hong, J. Y. Lee, P. Kim, and K.S. Kim, “Growth and applications of ultralong carbon nanotubes”, Patent No : US 8,080,281 B2, Registration Date : 2011.12.20, Application No:12/412,984, Country Registered: USA [USA Patent No, : PCT/US2007/020778 (60/848,023); (2007.9.27)]
4. V. Chandra, Y. Chun, J. W. Lee, I.-C. Hwang, K. S. Kim, “Hybrid materials comprising graphene and iron oxide, Method for manufacturing the same and Apparatus for treating waste water using the same”, Application No:13/279,291, Filing Date :2011.10.23, Country Registered: USA. “Hybrid materials comprising graphene and iron oxide, Method for manufacturing thereof and

Appratus for treating waste water using thereof ", Application No: 10-2010-0038705, Filing Date : 2010.04.26, Country Registered: Korea

5. W. Y. Kim and K. S. Kim, "Spin-valve devices based on graphene nanoribbons", [그래핀 나노리본을 이용한 스핀밸브 소자], Patent No: 10-0980680, Registration Date : 2010.09.01, Application No:10-2008-0077414, Country Registered: Korea
6. B. H. Hong, C.-W. Lee, and K.S. Kim, "Synthesis of organic nanotubes having suitable electrochemical and photochemical properties and synthesis of ultrathin nanowires using same as templates", European Patent No. (EP 1264919; 02 002 096.2, December 2002), Korean Patent No. (0439579, 2004), USA patent No. (6762331, 2004).
7. S. J. Lee and K. S. Kim, "Copyrighted S/W: POSMOL (POhang Sci-tech MOLecular modeling package)", Application No:2000-01-12-4239, Filing Date : 2000.06, Country Registered: Korea

Invited/Keynote/Plenary Talks and Organizing Chairs of International Conferences (since 1998)

1. "Structures and energetics of molecular clusters: Theoretical insights",
International Conference on "Chemistry of Small Manybody System",
Tokyo, Japan, Dec. 4-6, 1998.
2. "Ionophores and Receptors Using Cation-π Interactions: Collarenes",
CBM-IFOC Joint Symposium, Pohang, Korea, Nov. 27-28, 1998.
3. "Theoretical Studies on the Photochromic Activity of Diarylethylene Photoswitch Molecules",
8th Korea-Japan Joint Symposium: Molecular Science, Taejon, Korea, Jan. 7-9, 1999.
4. "Conformational vibrational effects of electrons and halide anions on water clusters",
Div. of Phys. Chem. 218th ACS Natl. Meeting, New Orleans, USA, Aug. 22-26, 1999.
5. "Conformational vibrational effects of electrons and halide anions on water clusters",
8th Asian Chemical Congress, Taipei, Taiwan, Nov. 21-24, 1999.
6. "Structures, energetics, and spectra of hydrated electrons and hydrated halide anions: Ab initio study",
Institute for Molecular Science, Okazaki, Japan, Dec. 19-22, 1999.
7. "Computational Investigation of Interaction Forces and their Importance in Molecular Recognition",
Workshop on Computational Chemistry, Hong Kong, Feb. 21-23, 2000.
8. "Nature of weakly bound complexes of π-systems: Comparison with H-bonded complexes",
Gordon Research Conference: Molecular Ionic Clusters (MIC 2000), Toulouse, France, April. 16-21, 2000.
9. "Design of Functional Molecular Systems Utilizing Interaction Forces in Chemical, Physical, and Biological Systems"
Computer Aided Molecular Design 2000 Symposium, Seoul, Korea, Jun. 20, 2000.
10. "Aqueous Clusters of Electrons, Halide Anions, and π Systems",
Water in Confined Geometries, Telluride, Colorado, USA, Jul. 30-Aug. 5, 2000.
11. "Theoretical Investigations of Ion solvation, Ionophore-Ion Interactions, and Receptor-substrate Interactions",
16th IUPAC Conference, Halifax, Canada, Aug. 6-11, 2000.
12. "Solvation Phenomena: Lessons from Theoretical Investigations of Aqueous Clusters of Electrons, Ions and π-Systems",
Symposium on Solvated Molecules and lons: from Clusters to Condensed Phases PacifiChem 2000, Honolulu, Hawaii, USA, Dec. 14-19, 2000.
13. "Self-assembled nanotubes and silver subnanowire arrays formed in and ambient solution phase",
The First Korean-Swedish Bilateal Symposium, Seoul, Korea, Nov. 5-7, 2001.
14. "Catalytic role of enzymes: partial proton shuttles and charge redistributions",
The 9th Korea-Japan Joint Symposium, Okazaki, Japan, Jan. 10-12, 2001.
15. [**plenary** talk] "De nove design of functional molecules, nanometerials, and nanodevices",
11th Current Trends for Computational Chemistry, Jackson State Univ. USA (Nov. 1-2, 2002).
16. [**keynote** speaker] "De nove design of functional nano-materials and molecular devices",
6th World Congress of Theoretically Oriented Chemists, Lugano, Switzerland (Aug. 4-9, 2002).

17. "Theoretical investigations of self-assembly in organic nanotube",
223rd Am. Chem. Soc. (ACS) National Meeting, Orlando, FL, USA (April 7-11, 2002).
18. "Theoretical Insights into the kaleidoscopic world of gas phase clusters and nanomaterials",
10th Korea-Japan Joint Symposium on Theoretical/Computational Chemistry, Postech (Jan 12-15, 2003).
19. "De nove design of functional nano-materials and molecular devices",
225th Am. Chem. Soc. (ACS) National Meeting, New Orleans, LA, USA (Mar. 23-27, 2003).
20. "Theory, Modeling and Simulation," International Conference on Materials for Advanced Technologies (ICMAT 2003), Singapore, 2003 (Dec. 10-13, 2003).
21. [**plenary** talk] "Nanomaterials and Moleculr Devices: Theoretical Exploration",
"Theory and Application of Computational Chemistry", Gyeongju, Korea (Feb. 15-20, 2004).
22. "Molecular Hosts for Anion Binding", 227th ACS Nat. Meeting, Anaheim, CA, USA (Mar.28-Apr.1, 2004).
23. [**plenary** talk] "Nanomaterials and molecular devices: theoretical and experimental explorations",
1st International Conference of Modern Trends in Physics, Cairo, Egypt (Apr. 4-9, 2004).
24. "Theoretical design and experimental realization of nanomaterials and nanodevices", Computer Modeling and Simulating Materials Nanoworld, Sicily, Italy (May 30-June 4, 2004).
25. [**plenary** talk] "Design of Functional Molecules and molecular devices", 15th Molecular Electronics and Devices Symposium, Postech (June 17-18, 2004).
26. "Theoretical Design of Ion Receptors", 228th ACS Nat. Meeting, Philadelphia, PA, USA (Aug.22-26, 2004).
27. "De nove design of function nano-materials and molecular devices",
7th World Congress of Theoretically oriented Chemists, Cape Town, South Africa (Jan. 15-21, 2005).
28. [**plenary** talk] "Functional molecules/materials and nanosensors: De Novo Design Approach based on Nanorecognition", 45th Sanibel Symposium, St. Simon's Island, GA, USA (Mar 5-11, 2005).
29. "Assembling Phenomenaof water-containing clusters and the design of ion-selective receptors", 229th ACS Nat. Meeting, San Diego, CA, USA (Mar 13-17, 2005).
30. "Design of ion selectivity receptors ", 3rd International Symposium on Calix-Supramolecular Chemistry, Dankook Univ., Seoul (Aug. 26, 2005).
31. "Ab initio study of structures and dynamics of molecular clusters toward the design of nanosensors", Symposium of Computational Quantum Chemistry; Methodology and Application, PacifiChem 2005, Honolulu, Hawaii, USA (Dec. 15-20, 2005).
32. "De novo design of functional nanomaterials based on nanorecognition", Symposium of Design of Nanomaterials and Nanodevices, PacifiChem 2005, Honolulu, Hawaii, USA (Dec. 15-20, 2005).
33. "Theoretical design of functional nanomaterials and nanodevices", 12th International Conference of Quantum Chemsitry (ICQC-2006), Kyoto, Japan (May 21-26, 2006).
34. "Structures, dynamics, and spectra of hydrated molecular clusters", Sendai International Conference, Sendai, Japan (May 29-30, 2006).
35. [**plenary** talk] "De Novo Design Approach Based on Nanorecognition: Functional Molecules/Materials and Nanosensors/Nanodevices", 18th International Conference on Physical Organic Chemistry (ICPOC-18), Warsaw, Poland (Aug. 20-25, 2006).
36. "Quantum Conductance of Silver Nanowires and Linearlization of Atomic Gold Chains" 234th ACS Nat. Meeting, Boston, USA (Aug. 19-23, 2007).
37. "Quantum Conductance of Magic Structures of Metal Nanowires and Design of Stable Linear Single Atomic Chains", 3rd APCTCC Meeting, Beijing, China (Sept. 22-26, 2007).
38. "Magic Structures and Quantum Conductance of Nanowires and Negative Differential Resistance of Molecular Electronic Devices", Korean Chem. Soc. Meeting, Taegu, Korea (Oct. 18-19, 2007).
39. [**plenary** talk] "Magic Structures and Quantum Conductance of Linear Ultrathin Nanowires and Negative Differential Resistance of Molecular Wires", 16th Current Trends for Computational Chemistry, Jackson State Univ. USA (Nov. 2-3, 2007).
40. "Quantum Conductance in Ultrathin Nanowires, Negative Differential Resistance in Molecular Wires, and Giant Magnetoresistance in Graphene Nanoribbon Devices", 1st International Conference of the Grand Challenge to Next Generation Integrated Naonoscience, Tokyo, Japan (June 3-7, 2008).
41. W. Y. Kim and K. S. Kim,* "Quantum Conductance of Ultrathin Nanowires, Negative Differential

Resistance in Molecular Wires, and Carbon-based Spin-valve Devices", Innovative Dynamic Studies of Materials at the Nanoscale, ECI, Gyeongju (June 30-July 3, 2008).
42. K. S. Kim, "Quantum Conductance of Ultrathin Nanowires, Negative Differential Resistance in Molecular Wires, and Carbon-based Spin-valve Devices", 14th International Symposium on the Physics of Semiconductors and Applications, (Special workshop of IPSA-2008, (Research Topics of GRL & GPP), Jeju (August 26-29, 2008).
43. K. S. Kim* and W. Y. Kim, "Super-Magnetoresitance in Graphene Nanoribbon Devices", 14th International Symposium on the Physics of Semiconductors and Applications, Jeju (Aug. 26-29, 2008).
44. "Super-Magnetoresistance in Graphene Nanoribbon Spin Valve Devices", WATOC 2008, Sydney, Australia (Sept. 14-19, 2008).
45. [**plenary** talk] W. Y. Kim and K. S. Kim,* "Quantum Conductance of Ultrathin Nanowires, Negative Differential Resistance in Molecular Wires, and Super-magnetoresitance of Graphene Nanoribbon Devices" Theory and Applications of Computational Chemistry (TACC2008), Shanghai, China (Sept. 23-27, 2008).
46. W. Y. Kim and K. S. Kim,* "Super-magnetoresitance in Graphene Nanoribbon Spin Valve Devices", Asian Magnetics Conference 2008, Busan (Dec. 10-13, 2008).
47. K. S. Kim, "Electron Transport in Nano-Devices", The International Conference on Simulations and Dynamics for Nanoscale and Biological Systems, Univ. of Tokyo, Japan (Mar, 4-6, 2009).
48. K. S. Kim, "De Novo Design of Molecular Electronics/Spintronics Devices", The 2nd Supercomputer Applications Workshop, Korea Univ., Seoul (May 26, 2009).
49. [**plenary** speaker] "Nanorecognition Based Design Approach: Functional Molecules/Materials and nanosensors/Nanodevices", The 19th Joint Seminar of the Busan Branch of the Korean Chemical Society and the Kyushu Branch of the Chemical Society of Japan, Busan (May 29, 2009).
50. K. S. Kim, "Molecular Electronics and Spintronics", The 2nd KIAS International Symposium on Recent Progress in Computer Simulations in Molecular Sciences, KIAS, Seoul (June 14-16, 2009).
51. K. S. Kim, "Electrode characteristics and super-magneto-resistance in graphene nanoribbon devices", KIAS Graphene Workshop, KIAS, Seoul (June 29- July 2, 2009).
52. K. S. Kim, "Synthesis of nanolens", Web lecture, Korea NanoTechnology Research Society (KoNTRS) (Sept 28, 2009).
53. K. S. Kim, "Nano-electronics, nano-spintronics, and nano-optics", Korea Supercomputing Conference 2009, KOEX, Seoul (Oct. 12-13, 2009).
54. K. S. Kim. "Nano-electronics/spintronics and nano-optics", Korean Chem. Soc. 2009 Fall Meeting (Oct. 29, 2009).
55. K. S. Kim, "Functional Molecules/Materials, Nano-electronics/spintronics, and Nano-optics", 4th SungAhm Symposium. Inha Univ., Incheon (Nov. 24, 2009).
56. K. S. Kim, "Molecular Assembly Based Nano-Electronics/Spintronics and Nano-Optics", Asian Pacific Conference of Theoretical and Computational Chemistry (APCTCC-4) Port Dickson, Malaysia (Dec. 21-23, 2009).
57. K. S. Kim, "Nanolens and Nano-Optics", Korean Optical Society Meeting, KAIST, Daejon (Jan 20-22, 2010).
58. K. S. Kim, Ulsan Chemistry Day, Ulsan (March 19, 2010).
59. K. S. Kim, "Nano-optics of nanolens." "Micro-Optics" conference, SPIE's International Symposium, Photonics Europe (EPE10), Brussels, Belgium (April 12-16, 2010)
60. K. S. Kim, "Theoretical design of functional molecules and nano-electronic/spintronic/optical materials", Molecular Quantum Mechanics 2010, Univ. of California, Berkeley, USA (May 24-29, 2010).
61. K. S. Kim, "Transport Phenomena in Molecular and Graphene Electronics/Spintronics", International Conference on Core Research and Engineering Science of Advanced Materials, Osaka Univ. Japan (May 30 – June 4, 2010).
62. [**keynote** speaker] K. S. Kim, "Present and Prospects of Nano-Chemistry Research", 2010 KRF Fundamental Science & Technology Research Workshop, Taejon (June 25, 2010).
63. K. S. Kim, Theoretical Understanding of Nano-electronics/spintronics and Nano-optics, International Conference in Honor of Prof. Jean-Marie, Namur, Belgium (July 5-8, 2010).

64. [**keynote** speaker] K. S. Kim, "Nano-sensing, Nano-electronics/spintronics, and Nano-optics", WCU 2nd International Symposium on IT Convergence Engineering, Postech, Pohang (Aug 19-20, 2010).
65. [**plenary** speaker] K. S. Kim, "Functional Molecules/Materials, Nano-electronics/spintronics, and Nano-optics", The Twentieth International Conference on Physical Organic Chemistry : ICPOC-20, Bexco, Busan (Aug 22-24, 2010).
66. [**keynote** speaker] K. S. Kim, International Union of Materials Research Societies - International Conference on Electronic Materials 2010 (IUMRS-ICEM2010), Computational Design for Next Generation Electronic Materials, Kintex, Seoul (Aug 24-27, 2010).
67. [**keynote** speaker] K. S. Kim, "Seeking Solutions to Mathematical and Physical Problems in Frontier Chemical Science", Inaugural symposium of Institute of Edge Science, Postech, Pohang (Sept 10, 2010).
68. K. S. Kim, "Carbon-based materials towards futuristic electronic devices and greener environments", Korean Carbon Society, Postech, Pohang (Nov. 5-6, 2010).
69. K. S. Kim, "Functional Nanomaterials, Nano-electronics/spintronics, and Nano-optics", Tokyo Tech – Tsinghua University Joint Symposium, Fuji-Yoshida, Japan (Nov. 11-13, 2010).
70. K. S. Kim, "Nanoscale optical lenses and plasmonic components toward integrated optical nano-devices", Nanotechnology Forum 2010, SAIT, Yongin (Nov. 12, 2010).
71. [**plenary** speaker] K. S. Kim, "Functional Molecules/Materials, Nano-electronics, and Nano-optics", NanoThailand: Nanotechnology for a Sustainable World, Bangkok, Thailand (Nov. 18-20, 2010).
72. K. S. Kim, "Study of electron transport phenomena in molecular electronics/spintronics based on density functional theory coupled to non-equilibrium Green function theory", Symposium #10: Computational Quantum Chemistry: Theory and Interactions with Experiment, PacifiChem 2010, Hawaii, USA (Dec. 15-20, 2010).
73. H. M. Lee, N. J. Singh, K. S. Kim, "Ab initio study of structures and dynamics of molecular clusters toward the design of functional molecules and nanomaterials", Symposium #81: Challenges and Solutions to Accurate Calculations on Large Molecular Systems, PacifiChem 2010, Hawaii, USA (Dec. 15-20, 2010).
74. [**plenary** speaker] "Functional Nanomaterials, Nano-electronics/spintronics, and Nano-optics", 2nd Nanoscience & Nanotechnology Global Research Lab Symposium (GRL-NT Symposium), Seoul (Feb 22., 2011)
75. [**plenary** speaker] K. S. Kim, "Functional Materials, Nanoptics, Molecular Electronics, and Ultrafast DNA Sequencing", Campus Asia Symposium, Shanghai Jia Tong Univ., Shanghai, China (March 10-12, 2011)
76. K. S. Kim, "Special Lecture on Nanoscience", Kyungbuk Science Education Center, Pohang (March 26, 2011).
77. K. S. Kim, "Molecular Electronics and Ultrafast DNA sequencing", Illumina Inc. San Diego, USA (April 5, 2011).
78. K. S. Kim, Mulliken Lecture, Univ of Georgia, Athens, USA (April 9, 2011).
79. [**plenary** speaker] K. S. Kim, "Ultrafast DNA sequencing", International Conference on Molecular Electronics and Devices (22nd IC ME&D) Pohang (May 19-20, 2011).
80. K. S. Kim, "Nanoelectronics/spintronics and Ultrafast DNA sequencing, International Conference of Materials for Advanced Technologies ICMAT 2011, Singapore (June 26-July 1)
81. K. S. Kim, "Ultrafast DNA Sequencing and Nano-Optics/Photonics", WATOC 2011, Satiago de Compostela, Spain (July 17-22, 2011).
82. K. S. Kim, "Molecular Electronics and ultrafast DNA sequencing", Fukui International Symposium for Theoretical Chemistry (FISTC), Kyoto, Japan (August 31-Sept 1, 2011).
83. K. S. Kim, "Molecular electronics and ultrafast DNA Sequencing", 7th Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII), Waseda Univ. Tokyo, Japan (Sept. 2-8, 2011).
84. K. S. Kim, Carbon-based Spintronics: *spin injection and manipulation in organic molecules, carbon nanotubes and graphene* (cspin11), Max Planck Institute for the Physics of Complex Systems, Dresden, Germany (Oct. 24-27, 2011).
85. [**plenary** speaker] K. S. Kim, Functional Molecules, Nano-Electronics/Spintronics/Photonics, and Ultrafast DNA Sequencing, 20th Conferences on Current Trends in Computational Chemistry (CCTCC), Jackson, Miss. USA (Oct. 27-29, 2011).

86. [**keynote** speaker] K. S. Kim, Molecular electronics and ultrafast DNA sequencing, SWOCS III. Pohang (Nov. 19, 2011).
87. [**keynote** speaker] K. S. Kim, Molecular Sensing, Nano-Electronics/Photonics, and Ultrafast DNA Sequencing, 5th Asian Pacific Conerence of Theoretical & Computational Chemistry (APCTCC), Rotorua, New Zealand (Dec. 9–13, 2011).
88. K. S. Kim, Nano- electronics/spintronics and ultrafast DNA sequencing, CECAM-Workshop, Univ. of Hong Kong (Dec. 12-16, 2011).
89. K. S. Kim, Graphene Based Ultrafast DNA Sequencing – 2-Dimensional Conductance, 243th ACS National Meeting , (San Diego, Mar 25-29, 2012).
90. K. S. Kim, Molecular Electronics Based Ultrafast DNA Sequencing, CECAM DNA workshop 2012, (Pisa, Italy June 11-13, 2012).
91. K. S. Kim, Efficient electron dynamics based on planewave-based real-time time-dependent density functional theory: vibronic electronic spectra, and coupled electron-nucleus dynamics, UCLA ICQC Satellite Symposium, QM and MD of Organic and Biological Reactivity, UCLA, LA, USA (June 21-23, 2012).
92. K. S. Kim, Nano- electronics/spintronics and ultrafast DNA sequencing, International Conference on Theoretical and High Performance Computational Chemistry 2012 (CT-HPCC12), Nanjing (July 8-11, 2012).
93. [**plenary** speaker] K. S. Kim, Molecular Electronics/Spintronics/Nano-Photonics, and Ultrafast DNA Sequencing, Nano Korea 2012 Symposium, 10th International Nanotech Symp & Nanoconvergence Expo, Coex, Seoul (Aug. 16-18, 2012).
94. K. S. Kim, Molecular Electronics, Nano-Photonics, and Ultrafast DNA Sequencing, Theory and Applications in Computational Chemistry, TACC-2012, Italy (Sept. 2-7, 2012).
95. K. S. Kim, Nature of various π interactions and harnessing to nano/bio systems**,** van der Waals Interactions in Complex Materials, CECAM HQ, Lausanne, Switzerland (Oct. 15-19, 2012).
96. K. S. Kim, Molecular Electronics Based Ultrafast DNA Sequencing, Pioneer Workshop on Nanopore 2013, Seoul Nat. Univ., Seoul (Feb. 21-23, 2013).
97. K. S. Kim, Various pi interactions for nano and bio systems, Accurate Characterization of Noncovalent Interactions: From Small Molecules to Supramolecular Chemistry, 245th ACS Nantional Meeting, New Orleans, USA (Apr. 7-11, 2013).
98. K. S. Kim, Molecular Electronics Spectroscopy and Fast DNA Sequencing, Novel Approaches to DNA Sequencing, Stockholm, Sweden (June 10-14, 2013).
99. [**keynote** speaker] K. S. Kim, Fano Resonance Driven Molecular Electronics Spectroscopy and Fast DNA Sequencing, APCTCC-6, Gyeongju, Korea (July 10-13, 2013).
100. K. S. Kim, Graphene for Electronics/Spintronics, Single Molecule Spectroscopy and Fast DNA Sequencing; Functionalized Graphene for Water Remediation, Fuel Cells, and Energy Materials/Devices 2D-Day Symposium: Graphene and beyond, Postech (Aug. 23, 2013).
101. [**keynote** speaker] K. S. Kim, Graphene for Electronics/Spintronics, Single Molecule Spectroscopy and Fast DNA Sequencing; International conference NANOCON´13, Brno, Czech. (October 16-18, 2013).
102. K. S. Kim, Remarkable oxygen reduction catalytic capacity of Pt nanoclusters and nanodendrites in genomic-DNA/reduced-graphene-oxide hybrid materials, International Conference on Small Science (ICSS 2013) Las Vegas, USA (Dec. 15-18, 2013).
103. K. S. Kim, Two dimensional Molecular Electronics Spectroscopy for Molecular Fingerprinting and DNA Sequencing, Pioneer Workshop 2014 on nanopore and nanofluidics –Physics and application as Biodevices, Osaka Univ. Japan (Feb. 7-8, 2014).
104. K. S. Kim, Eco-friendly Futuristic Energy Materials and Devices, UNIST BK21+ Symposium, Ulsan, Korea (Feb. 712-13, 2014).
105. K. S. Kim, Two Dimensional Molecular Electronics Spectroscopy for Molecular Fingerprinting, DNA Sequencing, and Cancerous DNA Recognition, International Workshop on Computational Quantum Chemistry in honor of Professor Jean-Marie Andre for his 70th anniversary, Tsinghua Univ., Beijing, China (March 31-April 1, 2014).
106. [**keynote** speaker] K. S. Kim, Two Dimensional Molecular Electronics Spectroscopy for Molecular Fingerprinting, DNA Sequencing, and Cancerous DNA Recognition, Korean Chemical Society (April 17, 2014).

107. K. S. Kim, Evaporation and condensation of metastable states of water, International Symposium on Frontiers of Theoretical and Computational Chemistry, Shenzhen, China (May 5- 6, 2014).
108. K. S. Kim, Remarkable oxygen reduction catalytic capacity of Pt nanoclusters and nanodendrites in Pt/DNA/reduced-graphene-oxide hybrid materials, Collaborative Conference on Materials Research (CCMR) 2014, Incheon (June 23-26, 2014).
109. [**plenary** speaker] K. S. Kim, Organic and Graphene Based Nanomaterials and Nanodevices, ICSM2014, Turku, Finland (June 30-July 5, 2014).
110. J. N. Tiwari, K. S. Kim, Energy delivery and enhanced catalytic activity by graphene and bio-organic hybrid materials, Graphene and Organic Hybrid Division, 15th International Conference on Organized Molecular Films (ICOMF 2014 (LB15)), Jeju (July 9-11, 2014).
111. K. S. Kim, Two Dimensional Molecular Electronics Spectroscopy for Molecular Fingerprinting and DNA Sequencing, WATOC 2014, Santiago, Chile, (Oct. 5-10, 2014).
112. K. S. Kim, Nano-Bio-Info fused science and technology, Educational program for new executives and maters, Samsung Electronics, Suwon, Korea (Jan. 28, 2015).
113. [**keynote** speaker] K. S. Kim, Electronic/spintronic devices, spectroscopy, and dynamics, 5th Symposium/Workshop of Computational Sciences (SWOCS5), Postech, Pohang, Korea (Feb. 3, 2015).
114. K. S. Kim, Nano-Bio-Info fused science and technology, 2014 Art-Design STEM Program, UNIST, Ulsan, Korea (Feb. 10, 2015).
115. [**plenary** speaker] K. S. Kim, Electronic/spintronic transport, spectroscopy, and dynamics, 15th International Congress of Quantum Chemistry (ICQC), Beijing, China (June 8-13, 2015).
116. [**keynote** speaker] K. S. Kim, Electronic Transport, Spectroscopy, and Dynamics, Current Status of Computational Chemistry , IUPAC-2015, 45th World Chemistry Congress, BEXCO, Busan (Aug 9-12, 2015).
117. K. S. Kim, Organic/Graphene Based Nanomaterials and Nanodevices 2015 ChemComm Symposia, UNIST, (Aug. 12-13, 2015).
118. K. S. Kim, Past, Present, and Future of Computational Quantum Chemistry: Korea vs World, Korean Chemical Society Meeting, Oct. 13-15, 2015.
119. K. S. Kim, Anisotropic noncovalent interactions in molecular assembly and collective properties in condensed phase, PacifiChem, Honolulu, Dec. 15-20, 2015.
120. K. S. Kim, Collective Properties and Liquid-Vapor Phases of Water, APCTCC7, Taiwan, Jan 25-28, 2016.
121. K. S. Kim, Electronic/Spintronic Transport, Spectroscopy, and Dynamics, 251st ACS National Meeting, San Diego, Mar. 13-17, 2016.
122. [**plenary** speaker] K. S. Kim, Organic/Graphene Based Nanomaterials and Nanodevices, 2nd International Conference on Smart Materials & Surfaces, SMS Korea, Incheon, 2016. Mar. 23-25, 2016.
123. K. S. Kim, Carbon/Graphene Based Nanomaterials/Nanodevices & Beyond: Electronic/Spintronic Transport & Spectroscopy, Low Dimensional Conference, Tabriz. May 22-23.2016.
124. K. S. Kim, Nano-Bio Fused Science: Nano-optics, Photonics and Energy Materials. Low Dimensional Conference, Tabriz. May 22-23.2016.
125. [**plenary** speaker] K. S. Kim, Carbon Based Nanomaterials/devices, Nanotech France, Paris, June 1-3, 2016.
126. K. S. Kim, Electron/spin transport in molecular electronics/spintronics devices, TACC 2016, Seattle, Aug. 25-Sep 3. 2016.
127. K. S. Kim, Graphene spintronics, Las Vegas, EMN Conference (Spintronics), Oct 11-13, 2016.
128. K. S. Kim, Graphene and Graphene Analogs Towards Opto-Electronic/Spintronic, Energy-Material, Sensing, and Medical Applications, 1st European Conference on Chemistry of Two-Dimensional Materials (Chem2DMat), Strasbourg, France, Aug. 22-26, 2017.
129. K. S. Kim, Graphene nanoribbon based electronics and spintronics, WATOC 2017, Munich, Germany, Aug. 27 - Sep. 1, 2017.
130. [**plenary** speaker] K. S. Kim, Interplay between theory & experiment towards novel optics/electronics/spintronics and efficient energy conversion, 22nd International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXII), Changsha/Zhanjiajie, China (Oct. 16-24, 2017).
131. [**Key-note** speaker] K. S. Kim, Interplay between theory & experiment towards novel optics/electronics/spintronics and efficient energy conversion, 25th International Conference on Current Trends

in Computational Chemistry (CCTCC), Jackson, USA (Nov. 10-11, 2017).
132. K. S. Kim, Electron/spin transport in nanodevices and electron/hole-phonon coupling in energy materials, APCTCC-8, Bombay, India (Dec. 15-17, 2017).
133. [**plenary** speaker] K. S. Kim, Metal doped carbon-shells/nanotubes for electrocatalysts and graphene nanoribbons for 2D molecular electronics spectroscopy, 122nd General meeting, Korean Chem. Soc., Daegu, Korea (Oct. 17-19, 2018).
134. K. S. Kim, Theoretical Design of Energy Materials - Electrocatalysts and Perovskite Solar Cells, ACS National Meeting, San Diego (Aug. 25-29, 2019).
135. K. S. Kim, Highly Efficient Electrocatalysts and Perovskite Solar Cells: Computer-Aided Design and Experimental Demonstration, 1st Kyoto Univ – UNIST joiny Symp on Chemistry & Mater. Science, Kyoto Univ. (Oct 24-26, 2019).
*** To be presented:
136. [**plenary** speaker] K. S. Kim, Molecular/ionic and/or e-photon/phonon interactions driven structural organization, phases, and collective properties of water and materials, ICMS 2019, Jeju, Korea, Nov. 3-6, 2019).
137. K. S. Kim, WATOC 2020, Vancouver, Canada (Aug. 16-21, 2020).
138. K. S. Kim, TACC 2020, Hokkaido Univ., Sapporo, Japan (Sept 7-12, 2020).
139. K. S. Kim, PacifiChem 2000, Hawaii (Dec. 15-20, 2020).
*** Invited talks at many foreign universities and national laboratories ***:
(1) "July-Aug. 2002": Max Plank Inst. (Mainz) Univ. Frankfurt Univ. Bonn; Acad. of Sci. Czech Republic.
(2) "Oct. 2002": Univ. Illinois (Urbana-Champaign); Northwestern Univ.
Univ. of Colorado, (Boulder); Pacific Northwest National Lab.
(3) "March 2003": Univ. Texas (Austin); Georgia Inst. Tech. (Phys); Univ. Pittsburgh; Yale Univ.
*** Invited talks at many Korean universities, nationa laboratories, industrial research centers ***:
(4) * Colloquium:
SNU, etc, etc…(a few times)
Gwangju Institute of Science and Technology (GIST): Dec. 18, 2008. ,
Quantum Conductance of Subnanowires, Negative Differential Resistance of Molecular Wires, and Super-magnetoresistance of Graphene Nanoribbon Devices,
Daegu Gyeogbuk Institute of Science and Technology (DGIST): Dec. 2012. Nov. 2016.
University of Dresden, Science Colloquium. Dec. 15, 2016..
MPI: Hamburg Phonon Science Colloquium. Dec. 16, 2016..

***** Organizing Chairperson of International Conferences**
1. [Organizing Chairman] The 9th Korea-Japan Joint Symposium, Okazaki, Japan (Jan. 10-12, 2001).
2. [Organizing Chairman] The 10th Korea-Japan Joint Symposium on Theoretical/Computational Chemistry, Postech (Jan 12-15, 2003).
3. {Organizing Chairman} "Theory and Application of Computational Chemistry", TACC 2004, Gyeongju, Korea (Feb. 15-20, 2004).
4. [Organizing board member) "Modeling and Simulating Materials Nanoworld", Sicily, Italy (May 30-June 4, 2004).
5. [Corresponding Organizer] Computational Quantum Chemistry Methodology and Application",
PacifiChem 2005, Honolulu, Hawaii, USA (Dec. 15-20, 2005).
6. [Co-Organizer] "Design of Nanomaterials and Nanodevices",
PacifiChem 2005, Honolulu, Hawaii, USA (Dec. 15-20, 2005).
7. {Organizing Chairpersons} "1st WCU Symposium/Workshop of Computational Sciences, Pohang, Korea (Nov. 21-22, 2009).
8. {Organizing Chairpersons} "2nd WCU Symposium/Workshop of Computational Sciences, Pohang, Korea (Oct. 31, 2010).
9. {Organizing Chairpersons} "3rd WCU Symposium/Workshop of Computational Sciences, Pohang, Korea (Nov. 19, 2011).

10. {Organizing Vice Chairperson} "Theory and Application of Computational Chemistry", TACC 2012, Pavia, Italy (Sep. 2-7, 2012).
11. {Organizing Chairpersons} "4th WCU Symposium/Workshop of Computational Sciences, Pohang, Korea (Nov. 17, 2012).
12. {Organizing Chairpersons} "6th Asia-Pacific Conference of Theoretical and Computational Chemistry, Gyeongju, Korea (July 10-13, 2013).