

Yong-Hoon Kim

Assistant Professor
Department of Materials Science and Engineering
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(updated: 2008.5.1)

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Education

- 1995.09–2000.07 **Ph.D. in Physics**, *University of Illinois at Urbana-Champaign, USA.*
Thesis advisor: Prof. Richard M. Martin
Thesis title: *"Density-functional study of molecules, clusters, and quantum nanostructures: development of nonlocal exchange-correlation approximations"*
- 1991.03–2000.02 **B.S. in Physics**, *Seoul National University.*

Professional Experience

Vocational

- 2006.08–present **Assistant Professor**, *Department of Materials Science and Engineering, University of Seoul.*
- 2004.04–2006.07 **Assistant Professor**, *School of Computational Sciences, Korea Institute for Advanced Study.*
- 2002.03–2004.03 **Postdoctoral Researcher**, *Materials and Simulation Center, California Institute of Technology.*
(with Prof. W. A. Goddard III)
- 2000.08–2002.02 **Postdoctoral Researcher**, *Lehrstuhl für Theoretische Chemie, Technische Universität München.*
(with Prof. A. Görling)

Miscellaneous

- 2002.09–2002.12 **Fellow**, *Institute for Pure and Applied Mathematics, University of California at Los Angeles.*
- 1995.08–2000.07 **Teaching and research assistant**, *Department of Physics, University of Illinois at Urbana-Champaign.*

Honors

- 2007 Best Lecture Note Awards, Association of Korean Engineering Deans
- 2006 Best Oral Presentation Awards, IEEE nanotechnology materials and devices conference
- 2002 IPAM fellowship for *Mathematics in Nanoscale Science and Engineering*, Institute for Pure and Applied Mathematics, UCLA, U.S.
- 2001 Humboldt Fellowship, Humboldt Foundation, Germany

Current Research Interests

- Nanowires and nanotubes
- Molecular and organic electronics
- Development of atomistic materials simulation methods and tools

Publications

(A) Refereed articles in journals (Bold face: More than 20 citation)

28. C. George, S. S. Jang, H. Yoshida, W. A. Goddard III, and Y.-H. Kim "Charge transport through polyene self-assembled-monolayers from multiscale computer simulations", J. Phys. Chem. C (to be published).
27. J. Kang, Y.-H. Kim, J. Bang, and K. J. Chang , "Defect-assisted electron tunneling and dielectric breakdown in ultra-thin SiO₂ layers", Phys. Rev. B **77**, 195321 (2008).
26. Y.-J. Kang, Y.-H. Kim, and K. J. Chang , "Electrical transport properties of nanoscale devices based on carbon nanotubes", Curr. Appl. Phys. (to be published).
25. Y.-H. Kim, "Toward numerically accurate first-principles calculations of nano-device charge transport properties: The case of alkane single-molecule junctions", J. Kor. Phys. Soc. **52**, 1181–1186 (2008).
24. G. I. Lee, J. K. Kang, and Y.-H. Kim, "Metal-independent coherent electron tunneling through polymerized fullerene chains", J. Phys. Chem. C **112**, 7029 (2008).
23. Y.-H. Kim, "Electrical and mechanical switching in a realistic [2]rotaxane device model" , J. Nanosci. Nanotech. **8** 4593–4597 (2008).
22. Y.-J. Kang, Y.-H. Kim, and K. J. Chang , "First-principles study of the electrical conductance of telescopically aligned carbon nanotubes", Phys. Rev. B **76**, 205441 (2007).
21. Y.-J. Kang, J. Kang, Y.-H. Kim, K. J. Chang, "First-principles approach to the electron transport and applications for devices based on carbon nanotubes and ultrathin oxides", Comput. Phys. Commun. **177**, 30–33 (2007).
20. Y.-H. Kim and W. A. Goddard III, "Efficiency of π - π tunnelling in [2]rotaxane molecular electronic switches", J. Phys. Chem. C **111**, 4831 (2007).
19. D. Sung, S. Hong, Y.-H. Kim, N. Park, S. Kim, S. L. Maeng, K.-C. Kim, "First-principles study of the effect of the water adsorption on the carbon nanotube field effect transistor", Appl. Phys. Lett. **89**, 243110 (2006). [Note: selected for the December 25, 2006 issue of Virtual Journal of Nanoscale Science & Technology]
18. Y.-H. Kim, J. Tahir-Kheli, P. A. Schultz, and W. A. Goddard III, "First-principles approach for the charge transport characteristics of monolayer molecular electronic devices: Application to hexanedithiolate devices", Phys. Rev. B **73**, 235419 (2006). [Note: selected for the July 4, 2006 issue of Virtual Journal of Nanoscale Science & Technology]
17. Y.-H. Kim, S. S. Jang, and W. A. Goddard III, "Possible performance improvement in [2]catenane molecular electronic switches", Appl. Phys. Lett. **88**, 16311 (2006).
16. S. Soares, S. Dasgupta, Y.-H. Kim, C. B. Musgrave, P. A. Schultz, W. A. Goddard III, "Density functional theory study of the geometry, energetics, and reconstruction process of Si(111) surfaces", Langmuir **21**, 12404 (2005).
15. S. S. Jang, Y. H. Jang, Y.-H. Kim, W. A. Goddard III, J. W. Choi, J. R. Heath, B. W. Laursen, A. H. Flood, J. F. Stoddart , S. S. Jang, Y. H. Jang, W. A. Goddard III, "Molecular dynamics simulations of amphiphilic bistable [2]rotaxane Langmuir monolayer at air/water interface", J. Am. Chem. Soc. **127**, 14804 (2005).
14. Y.-H. Kim, S. S. Jang, W. A. Goddard III, "Conformations and charge transport characteristics of biphenyldithiol self-assembled-monolayer molecular electronic devices: A multiscale computational study", J. Chem. Phys. **122**, 244703 (2005). [Note: selected for the July 11, 2005 issue of Virtual Journal of Nanoscale Science & Technology; erratum: **123**, 169902 (2005)]
13. Y.-H. Kim, S. S. Jang, Y. H. Jang, W. A. Goddard III, "First-principles study of the switching mechanism of [2]catenane molecular electronic devices", Phys. Rev. Lett. **94**, 156801 (2005). [Note: selected for the May 2, 2005 issue of Virtual Journal of Nanoscale Science & Technology]
12. S. S. Jang, Y. H. Jang, Y.-H. Kim, W. A. Goddard III, A. H. Flood, B. W. Laursen, H.-R. Tseng, J. F. Stoddart, J. O. Jeppesen, J. W. Choi, D. W. Steurman, E. Delonno, J. R. Heath, "Structure and properties of self-assembled monolayers of bistable [2]rotaxanes on Au (111) surfaces from molecular dynamics simulations validated with experiment", J. Am. Chem. Soc. **127**, 1563 (2005).

11. Y. H. Jang, S. Hwang, Y.-H. Kim, S. S. Jang, W. A. Goddard III, "Density-functional theory studies of the [2]rotaxane component of the Stoddard-Heath molecular switch", J. Am. Chem. Soc. **126**, 12636 (2004).
10. Y.-H. Kim, M. Städele, and A. Görling, "Optical excitations of Si by time-dependent density-functional theory based on the Kohn-Sham exact-exchange band structure", Int. J. Quant. Chem. **91**, 257 (2003).
9. Y.-H. Kim and A. Görling, "Excitonic optical spectrum of semiconductors obtained by time-dependent density-functional theory with the exact-exchange kernel", Phys. Rev. Lett. **89**, 096402 (2002).
8. Y.-H. Kim and A. Görling, "Exact Kohn-Sham exchange kernel for insulators and its long-wavelength behavior", Phys. Rev. B **66**, 035114 (2002).
7. I.-H. Lee, Y.-H. Kim, and K.-H. Ahn, "Electronic structure of ellipsoidally deformed quantum dots", J. Phys.: Condens. Matter **13**, 1987 (2001).
6. Y.-H. Kim, I.-H. Lee, and R. M. Martin, "Object-oriented construction of a multigrid electronic-structure code with Fortran 90", Comput. Phys. Commun. **131**, 10 (2000).
5. I.-H. Lee, Y.-H. Kim, and R. M. Martin, "One-way multigrid method in electronic-structure calculations", Phys. Rev. B **61**, 4397 (2000).
4. Y.-H. Kim, I.-H. Lee, S. Nagaraja, J.-P. Leburton, R. Q. Hood, and R. M. Martin, "Two-dimensional limit of exchange-correlation energy functional approximations", Phys. Rev. B **61**, 5202 (2000).
3. I.-H. Lee, K.-H. Ahn, Y.-H. Kim, R. M. Martin, and J.-P. Leburton, "Capacitive energies of quantum dots with hydrogen impurity", Phys. Rev. B **60**, 13720 (1999).
2. Y.-H. Kim, M. Städele, and R. M. Martin, "Density-functional study of small molecules within the Krieger-Li-Iafate approximation", Phys. Rev. A **60**, 3633 (1999).
1. S. Nagaraja, P. M., V.-Y. Thean, J.-P. Leburton, Y.-H. Kim, and R. M. Martin, "Shell-filling effects and Coulomb degeneracy in planar quantum-dot structures", Phys. Rev. B **56**, 15752 (1997).

(B) Others

3. Y.-H. Kim and W. A. Goddard III, "First-principles study of charge transport across alkene thiolate self-assembled monolayers", in *Proceedings of IEEE Nanotechnology Materials and Devices Conference* (2006).
2. Y.-H. Kim, "Density-functional study of molecules, clusters, and quantum nanostructures: development of nonlocal exchange-correlation approximations", Ph. D. thesis, University of Illinois at Urbana-Champaign (2000).
1. Y.-H. Kim, I.-H. Lee, and R. M. Martin, "Density-functional study of the hydrogen-bonded water cluster $H_5O_2^+$ ", in *AIP conference proceedings 501: Stochastic Dynamics and Pattern Formation in Biological and Complex Systems*, 366-372 (AIP, 2000).

Presentations

- 2008.10.1, Kunkuk University, Seoul (seminar).
- 14th International Symposium on the Physics of Semiconductors and Applications, 2008.8.26~29, Jeju (talk).
- Nano Korea 2008, 2008.8.27~29, Seoul (poster).
- Materials Research Society 2007 Fall Meeting, 2007.11.26~30, Boston, U.S. (invited talk).
- 2008.7.21, Kumoh National University, Gumi (tutorial).
- 2008.4.4, Kyung Hee University, Seoul (seminar).
- American Physical Society 2008 March Meeting, 2008.3.10~14, New Orleans, U.S. (talk).
- Materials Research Society 2007 Fall Meeting, 2007.11.26~30, Boston, U.S. (invited talk).

- *The 4th Conference of the Asian Consortium on Computational Materials Science*, 2007.9.13~16, KIST, Seoul (talk).
- *The 18th International Conference on Molecular Electronics and Devices*, 2007.5.10~11, ETRI, Daejeon (invited talk).
- *The 2nd Workshop on Molecular Computation*, 2007.2.12~13, KIAS, Seoul (invited talk).
- 2006.11.27, National Taiwan University, Taipei, Taiwan (seminar).
- *Supercomputing Korea 2006*, 2006.11.20~21, KIAS, Seoul (invited talk).
- 2006.11.16, Chunbook National University, Jeonju (seminar).
- *IEEE Nanotechnology Materials and Devices Conference*, 2006.10.22~25, Gyeongju (talk).
- *Nanotube 06*, 2006.6.18~23, Nagano, Japan (poster).
- *Korean Physical Society Spring Meeting*, 2006.4.20~21, Phoenix Park, Pyungchang (invited talk).
- 2006.3.28, KAIST, Daejeon (colloquium).
- *American Physical Society March Meeting*, 2006.3.13~17, Baltimore, MD, U.S. (talk).
- *Asian Workshop on Surface Nano-science*, 2006.2.9~11, Phoenix Park, Pyungchang (tutorial).
- 2005.11.16, Seoul National University, Seoul (seminar).
- *8th Asian Electronic Structure Workshop*, 2005.10.29~11.1, Shanghai, China (invited talk).
- 2005.9.29, KAIST, Daejeon (seminar).
- *2nd KIAS Workshop on Electronic Structure Calculations*, 2004.6.13~15, KIAS, Seoul (lecture).
- 2005.5.18, Hanyang University, Seoul (seminar).
- *Nano-SoC lecture series*, 2005.4.30, Korea University, Seoul (seminar).
- *American Physical Society March Meeting*, 2005.3.21~25, Los Angeles, CA (talk).
- 2004.11.19/30, Samsung Advanced Institute of Technology, Suwon, Korea (lectures).
- *7th Asian Electronic Structure Workshop*, 2004.11.1~3, Taipei, Taiwan (poster).
- 2004.10.5, Ewha woman's university, Seoul (seminar).
- *1st KIAS Workshop on Electronic Structure Calculations*, 2004.9.13, KIAS, Seoul, Korea (seminar).
- 2004.7.13, Samsung Advanced Institute of Technology, Suwon, Korea (seminar).
- 2004.7.5, Postech, Pohang, Korea (seminar).
- 2004.6.29, Electronics and Telecommunications Research Institute, Daejun, Korea (seminar).
- *IPAM Nano Reunion Conference*, 2004.6.8, Arrowhead, CA, U.S. (invited talk).
- 2004.6.1, Seungkyunkwan University, Suwon (seminar).
- *American Physical Society March Meeting*, 2004.3.22~26, Montreal, Canada (talk).
- *2003 U.S.-Korea Conference on Science, Technology, and Entrepreneurship*, 2003.8.8~10, 2003, California Institute of Technology, Pasadena, CA (talk).
- 2003.5.19, Korea Institute for Advanced Study, Seoul (seminar).
- 2002,10.18, Institute for Pure and Applied Mathematics, University of California at Los Angeles, Los Angeles, CA, U.S. (seminar).

- *Sandia Workshop on Quantum Mechanical Techniques: Exchange Correlation Functionals in Density Functional Theory*, 2002.8.14~16, 2002, Albuquerque, New Mexico (invited talk).
- 2002.7.25, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany (seminar).
- 2002.2.28, Seoul National University, Seoul, Korea (seminar).
- 2001.11.17, University of Würzburg, Germany (seminar).
- *9th International Conference on the Applications of the Density Functional Theory in Chemistry and Physics*, 2001.9.10~14, San Lorenzo de El Escorial, Madrid, Spain (poster).
- 2001.8.10, Lawrence Livermore National Laboratory, Livermore, CA, U.S. (seminar).
- 2001.6.6, University of Illinois at Urbana-Champaign, Urbana, IL, U.S. (seminar).
- *International Workshop on Artificial Atoms and Related Finite Fermion and Boson Systems*, 2000.9.24~10.6, Trento, Italy (invited talk).
- *Psi-k 2000 Conference*, 2000.8.22~26, Schwäbisch Gmünd, Germany (talk).
- 2000.7.27, Seoul National University, Seoul (seminar).
- *12th Electronic Structure Workshop*, 2000.5.19~22, Atlanta, GA, U.S. (poster).
- *American Physical Society March Meeting*, 2000.3.20~24, Minneapolis, MN, U.S. (talk).
- *11th Electronic Structure Workshop*, 1999.5.21~24, University of Illinois, Urbana, IL, U.S. (poster).
- *American Physical Society March Meeting*, 1999.3.20~26, Atlanta, GA, U.S. (talk).
- *APCTP International Workshop on Stochastic Dynamics and Pattern Formation in Biological Systems*, 1999.7.7~10, Korea University, Seoul (poster).
- *10th Electronic Structure Workshop*, 1998.5.29~6.1, University of Pennsylvania, Philadelphia, PA, U.S. (poster).
- *American Physical Society March Meeting*, 1998.3.16~20, Los Angeles, CA, U.S. (talk).
- *9th Electronic Structure Workshop*, 1997.5.31~6.2, Cornell University, Ithaca, NY, U.S. (poster).
- *American Physical Society March Meeting*, 1997.3.17~21, Kansas City, MO, U.S. (talk).