Curriculum Vitae

Name:	Yong-Hyun Kim
Birth:	(date) 25 March 1972 (place) Daejeon, Korea
Address:	National Renewable Energy Laboratory 1617 Cole Boulevard Golden, Colorado 80401 U.S.A
E-mail:	ykim@nrel.gov
Web:	http://dielc.kaist.ac.kr/yonghyun
Phone:	+1-303-384-6465
Fax:	+1-303-384-6655

EDUCATION

- B.S. in Physics, Korea Advanced Institute of Science and Technology, Daejeon, Korea, 1990-1997 (including the mandatory military service)
  - Student of Prof. Dojun Youm, "Calculation on S/F boundary problems using the Radovic method"
- M.S. in Physics, Korea Advanced Institute of Science and Technology, Daejeon, Korea, 1997-1999
  - Student of Prof. Kee Joo Chang, "First-principles study on the Coulomb pseudopotential of Pd and PdH"
- Ph.D. in Physics, Korea Advanced Institute of Science and Technology, Daejeon, Korea, 1999- Feb. 2003
  - Student of Prof. Kee Joo Chang, "Theoretical study on the physical properties of carbon nanotubes"
- Post-Doc. in National Renewable Energy Laboratory, Golden, Colorado 80401, USA, Mar. 2003- present

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HONORS

- A Bronze Medal in the Korean Mathematical Olympiad, 1989
- A Best Poster Award in April meeting of the Korean Physical Society, 2001
  - Yong-Hyun Kim and K. J. Chang, "Coherent electron transport in carbon nanotube field effect transistors"

- A Certificate of Appreciation in the Nanotube 2001- Workshop, 2001
  - "The web man"
- A Best Poster Award in April meeting of the Korean Physical Society, 2002
  - Yong-Hyun Kim, In-Ho Lee, and K. J. Chang, "Finite temperature action-derived molecular dynamics simulations for molecular transformations of C_{60}"

EXPERIENCE

- Teaching Assistant at Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon, Korea, Mar. 1998- Feb. 2000
  - General Physics (undergraduate level), Quantum Mechanics (graduate level)
- Research Associate at Supercomputing Center, Daejeon, Korea, Jul. 2001- Jan. 2002
- Research Associate at Korea Research Institute of Standards and Science, Daejeon, Korea, Aug. 2002- Dec. 2002

RESEARCH EXPERIENCE

- Theoretical calculation for superconducting properties
  - Green-Function approach for the proximity effects in superconducting/ferromagnetic multilayers
  - First-principle calculation of electron-electron interaction as a parameter of superconductivity (Coulomb pseudopotential μ^*, which is usually assumed to be 0.1) in Pd and PdH
  - Coulomb pseudopotential of MgB_2
- *Ab initio* pseudopotential density-functional calculation with plane-wave, real-space grid, or LCAO (Linear Combination of Atomic Orbitals) basis set
  - Dielectric response function and screening effect in Pd and PdH
  - Electronic structure of finite-length carbon nanotubes
  - Electronic structure modification by radial deformation or transverse electric fields in carbon, BN, and BC_3 nanotubes
  - Occurrence of ferromagnetism in C/BN heterostructured nanotubes
  - Magnetic instability in a defective C_{60}
  - Electronic and magnetic properties in Ti-coated single-wall carbon nanotubes

- Quantum conductance calculation with a LCAO-type basis
  - Back scattering in large-diameter carbon nanotubes in the presence of transverse electric fields with one-orbital tight-binding Hamiltonian
  - Coherent electron transport in carbon nanotube field-effect transistors with one-orbital tight-binding Hamiltonian
  - Spin-dependent electron transport in the Ferromagnetic Kondo Hamiltonian for mixed phase manganites
  - Spectral correlation in incommensurate double-wall carbon nanotubes via the nearest-level statistics
- Action-derived molecular dynamics with the Tersoff's empirical potential and tight-binding Hamiltonian
  - Development of new molecular dynamics methods for rare-event study with classical action
  - Application to the Stone-Wales defect formation in C_{60}
  - Fullerene coalescence
- Nudged Elastic Band calculation
  - Activation energy barrier for the Stone-Wales defect formation in C_{60}
- Programming Experience and Computer Skills
  - Dielectric Matrix calculation with elimination of unoccupied-states summation
  - Conductance calculation with a LCAO basis set
  - Conjugate Gradient local minimization for action-derived molecular dynamics
  - Monte Carlos simulation for the two-dimensional Ising model
  - Simulated Annealing
  - Matrix diagonalization and inversion with LAPACK (serial) or SCALAPACK (parallel) routines
  - Working on IBM SP3, IBM-POWER4, Cray-T3E, Cray-C90, NEC-SX5, and Compaq-SMP supercomputers, and Origin 200 workstation
  - Code: PARATEC, SIESTA, Real-Space Multigrid Electronic Structure Calculation (with Norm-Conserving PS), PW-SCF (with Ultra-Soft PS, preliminarily), etc.
  - Programming language: FORTRAN90, C, and MPI

RESEARCH INTEREST

- Excitation properties of solids

- New physical properties of composite nano-systems
- Transport properties of quantum-functional devices
- Dynamical simulation of chemical reaction, atomic diffusion, molecular conformational change, and so on
- Defects in semiconductors and quantum Monte Carlos calculation

Since the initial stage of my physics life, I have been so interested in the superconducting phenomena and attracted to the beauty of the BCS theory. The starting point was a theoretical consideration in the superconductivity field. For a bachelor degree, I solved a group of linear equations from the Green functions of superconducting states in superconducting/ferromagnetic multilayer systems. I found that spin-orbit scattering effects suppress the proximity effects at the interface, and reported it at Physical Review. For a master degree, I joined with Prof. Kee Joo Chang's group and learned the first-principles calculation technique for the ground state of real materials. Since I had much interest in superconductivity, Prof. Chang recommended to me the calculation of the Coulomb pseudopotential μ^* of Pd and PdH, that is, a parameter of superconductivity regarding electron-electron interaction, associated with excitation properties of the materials. The dielectric matrix that I calculated with first-principles approach contains the excitation information. For the dielectric matrix of a large cell, I programmed an iterative matrix inversion technique and conduction-band elimination technique in the calculation of the independent polarizability. So I have continual interest in the excitation properties of solids through dielectric response function and GW quasiparticle self-energy calculation.

For a Ph. D. degree, I have been really engaged in carbon nanotubes and nanostructured materials. At that time, nobody in Prof. Chang's group was working on nanotube systems. As a start point, we focused on mechanical deformation of carbon nanotubes and its effects on electronic properties, using the first-principles pseudopotential approach. Then, we found that the electronic structure, especially the band gap, can be modified systematically when the cross-section of carbon nanotubes is changed with an elliptical shape. A metallic nanotube can be a semiconducting one in the deformation, and vise versa. In the collaboration with Prof. Steven G. Louie at UC Berkeley, we examined the same possibility in BN and BC_3 nanotubes, which are more important in optical applications. We also found that the transverse electric fields modify electronic structure of carbon nanotubes including band-gap closure in semiconducting tubes. Next, we studied magnetic properties of nanostructured systems with the local spin-density functional formulation. We found, in collaboration with Prof. David Tomanek at Michigan State University, magnetic instabilities in C/BN composite nanotubes and defective C_{60} molecules, which are truly *s-p* electron systems. So expectation of new physical properties in new (composite) nanostructured systems based on the first-principles density-functional formulation is one of my major future works.

In order to investigate transport properties of nanostructures, I calculated quantum conductance following the Landauer-Büttiker formalism with LCAO-type Hamiltonians. With a simple one-orbital tight-binding model, I examined transport characteristics of carbon nanotube devices under influence of external gate voltages or transverse electric fields. I also derived, in collaboration with Dr. H.S. Yi at Supercomputing center in Korea, the spin-dependent conductance of the ferromagnetic Kondo model for spin devices of mixed

phase manganites. With Dr. K.-H. Ahn at Seoul National University, I investigated transport properties of incommensurate double-wall carbon nanotubes with spectral analysis techniques, and found that, depending on the doping level, the transport can be diffusive or ballistic. Since the SIESTA code offers LCAO-type Hamiltonian based on density-functional formulation, I can do *ab initio* conductance calculation for general devices.

Recently, I have developed a new molecular dynamics method, in collaboration with Dr. In-Ho Lee at Korea Research Institute of Standards and Science in Daejeon, utilizing classically-defined action for N-particle systems, originally proposed by Dr. D. Passerone and Dr. M. Parrinello at Max Planck Institute, Stuttgart. With the Nudged Elastic Band technique for estimating a transition state, this method can serve as an important tool in the study of rare events, such as chemical reaction, atomic diffusion, and molecular conformational change. We applied the method to the study of the Stone-Wales defect formation in a C_{60} molecule and the fullerene (C_{60}) coalescence with a tight-binding model.

Since many colleagues in Prof. Chang's group are involved in research on defect problems in semiconductors, I am very familiar with the problems. So, I also have much interest in problem of semiconductors, such as doping problem in wide-gap semiconductors and alloying problem with nitrogen. In private, I passed a course work of the Monte Carlo method. I am very interested in quantum Monte Carlo calculation of physical properties of solids and molecules.

PUBLICATIONS

1. Sangjun Oh, **Yong-Hyun Kim**, and Do Jun Youm, *Spin-orbit scattering effect on the oscillatory T_c of superconductive and magnetic multilayers*, Sae Mulli (The Korean Physical Society) **38**, 199 (1998).

2. Chan-Jeong Park, **Yong-Hyun Kim**, and K. J. Chang, *Band-gap modification by radial deformation in carbon nanotubes*, Phys. Rev. B **60**, 10656 (1999).

3. **Yong-Hyun Kim**, Chan-Jeong Park, and K. J. Chang, *Subbands in carbon nanotubes under radial deformation*, J. Korean Phys. Soc. **37**, 85 (2000).

4. Sangjun Oh, **Yong-Hyun Kim**, D. Youm, and M. R. Beasley, *Spin-orbit scattering effect on the oscillatory T_c of superconductive/magnetic multilayers*, Phys. Rev. B **63**, 52501 (2001).

5. **Yong-Hyun Kim**, H.-S. Sim, and K. J. Chang, *Electronic structure of collapsed C, BN, and BC_3 nanotubes*, Current Applied Physics **1**, 39 (2001).

6. **Yong-Hyun Kim**, K. J. Chang, and S. G. Louie, *Electronic structure of radially deformed BN and BC_3 nanotubes*, Phys. Rev. B **63**, 205408 (2001).

7. **Yong-Hyun Kim**, K.J. Chang, and S. G. Louie, *Band-gap modification by radial deformation in C, BN, and BC_3 nanotubes*, Proceedings of the 25th International Conference on the Physics of Semiconductors (Park II), 1645 (2001).

8. **Yong-Hyun Kim** and K. J. Chang, *Subband mixing rules in circumferentially perturbed carbon nanotubes: Effects of transverse electric fields*, Phys. Rev. B **64**, 153404 (2001).

9. Dong-Hee Kim, **Yong-Hyun Kim**, and K. J. Chang, *Conductance calculation on carbon nanotube devices*, Sae Mulli (The Korean Physical Society) **44**, 149 (2002).

10. **Yong-Hyun Kim** and K. J. Chang, *Electron transport through quantum-dot states of n-type carbon nanotubes*, Appl. Phys. Lett. **81**, 2264 (2002).

11. **Yong-Hyun Kim**, In-Ho Lee, and K.J. Chang, *Action-derived molecular dynamics simulation on the coalescence of C_{60} molecules*, Proceedings of the 26th International Conference on the Physics of Semiconductors, to be published (2002).

12. K.-H. Ahn, **Yong-Hyun Kim**, J. Wiersig, and K. J. Chang, *Spectral correlation in incommensurate multi-walled carbon nanotubes*, cond-mat/0208278, Phys. Rev. Lett. **90**, 026601 (2003).

13. **Yong-Hyun Kim**, I.-H. Lee, K. J. Chang, and Sangsan Lee, *Dynamics of fullerene coalescence*, cond-mat/0211059, Phys. Rev. Lett. **90**, 065501 (2003).

14. J. Choi, **Yong-Hyun Kim**, K. J. Chang, and D. Tomanek, *Itinerant ferromagnetism in heterostructured C/BN nanotubes*, Phys. Rev. B **67**, 125421 (2003).

15. J. Choi, **Yong-Hyun Kim**, K. J. Chang, *Ferromagnetism in ultrathin films and nanowires of Ti on graphene sheet and carbon nanotubes*, Phys. Rev. Lett., submitted (2003).

16. S. Bandow, K. Hirahara, T. Kawai, Y. Miyamoto, **Yong-Hyun Kim**, K. J. Chang, S. Iijima, *Diameter adjustment effect in double-wall nanotubes developed from peapods*, Phys. Rev. B, submitted (2003).

17. **Yong-Hyun Kim**, J. Choi, K. J. Chang, and D. Tomanek, *Defective fullerenes and nanotubes as molecular magnets: An* ab initio *study*, Phys. Rev. Lett., to be submitted (2003).

TALKS AND PRESENTATIONS

1. Sangjun Oh, **Yong-Hyun Kim**, and D. Youm, *Spin-orbit scattering effect on the oscillatory T_c superconductive/magnetic multilayers*, KPS Meeting, Seoul (Korea), April, 1998.

2. **Yong-Hyun Kim**, Young-Gu Jin, and K.J. Chang, *First-principles study of the dielectric response functions and the coulomb pseudopotentials of Pd and PdH*, KPS Meeting, Junju (Korea), October, 1998.

3. **Yong-Hyun Kim**, Young-Gu Jin, and K.J. Chang, *Electronic structures of elastically deformed carbon nanotubes*, KPS Meeting, Seoul (Korea), April, 1999.

4. **Yong-Hyun Kim**, Chan-Jeong Park, and K. J. Chang, *Electronic structure of flattened carbon nanotubes*, CMS Symposium, Taejon (Korea), July, 1999.

5. Chan-Jeong Park, **Yong-Hyun Kim**, and K. J. Chang, *Band gap opening and closure in radially deformed carbon nanotubes*, KPS Meeting, Pusan (Korea), October, 1999.

6. **Yong-Hyun Kim**, Chan-Jeong Park, and K. J. Chang, *Electronic structure of flattened chiral carbon nanotubes*, KPS Meeting, Pusan (Korea), October, 1999.

7. **Yong-Hyun Kim**, Chan-Jeong Park, and K. J. Chang, *Electronic structure of flattened carbon nanotubes*, The 2nd Korea-Japan Joint Workshop on Electronic Structure Calculations, Seoul (Korea), November 1-3, 1999.

8. **Yong-Hyun Kim**, Chan-Jeong Park, and K. J. Chang, *Electronic structure of carbon nanotubes under flattening deformation*, Symposium 2000 on Theoretical Solid State Physics, Taejon (Korea), January, 2000.

9. **Yong-Hyun Kim**, K.J. Chang, and S. G. Louie, *Band-gap modification in BN and BC_3 nanotubes: A first principle study*, KPS Meeting, Seoul (Korea), April, 2000.

10. K. J. Chang, **Yong-Hyun Kim**, and H.-S. Sim, *Electronic structure of collapsed C, BN, and BC_3 nanotubes*, International Workshop on Quantum Transport in Synthetic Metals II, Seoul (Korea), August 28-31, 2000.

11. **Yong-Hyun Kim**, K.J. Chang, and S. G. Louie, *Band-gap modification by radial deformation in BN and BC_3 nanotubes*, The 25th International Conference on the Physics of Semiconductors, Osaka (Japan), September 17-22, 2000.

12. **Yong-Hyun Kim** and K.J. Chang, *Coherent electron transport in carbon nanotube field effect transistors*, KPS Meeting, Seoul (Korea), April, 2001. **Received the best poster award.**

13. **Yong-Hyun Kim** and K.J. Chang, *Band gap modification by circumferentially perturbing potentials in carbon nanotubes*, International Workshop on the Science and Application of Nanotubes (Nanotube 2001), Potsdam (Germany), July 22-25, 2001. **Received an award for helping web work.**

14. Hongsuk Yi, **Yong-Hyun Kim**, and K.J. Chang, *Phase separation and pseudogap in mixed phase manganites*, KMS Meeting, Suwon (Korea), October, 2001.

15. **Yong-Hyun Kim** and K.J. Chang, *Band gap modification and back scattering in carbon nanotubes under transverse electric fields*, KPS Meeting, Kwangju (Korea), October, 2001.

16. Hongsuk Yi, **Yong-Hyun Kim**, and K.J. Chang, *Pseudogap and conductance in mixed-phase manganites*, KPS Meeting, Kwangju (Korea), October, 2001.

17. **Yong-Hyun Kim**, In-Ho Lee, and K.J. Chang, *Finite temperature action-derived molecular dynamics simulations for molecular transformations of C_{60}*, KPS Meeting, Pusan (Korea), April, 2002.

18. In-Ho Lee, **Yong-Hyun Kim**, J. Lee, and K.J. Chang, *Finite-temperature action-derived molecular dynamics in rare event simulations*, KPS Meeting, Pusan (Korea), April, 2002.

19. J. Choi, **Yong-Hyun Kim**, K.J. Chang, and D. Tomanek, *Magnetic ordering based on the Hund's rule in C/BN superlattice nanotubes*, KPS Meeting, Pusan (Korea), April, 2002.

20. J. Choi, **Yong-Hyun Kim**, K.J. Chang, and D. Tomanek, *Heterostructured C/BN nanotubes as one-dimensional magnets*, International Workshop on Quantum Transport in Synthetic Metals III, Seoul (Korea), May, 2002.

21. **Yong-Hyun Kim**, In-Ho Lee, and K.J. Chang, *Fullerene coalescence in fullerene-aided nanotube growth*, International Workshop on the Science and Application of Nanotubes (Nanotube 2002), Boston (USA), July, 2002.

22. J. Choi, **Yong-Hyun Kim**, K.J. Chang, and D. Tomanek, *Occurrence of ferromagnetism in heterostructured C/BN nanotubes*, International Workshop on the Science and Application of Nanotubes (Nanotube 2002), Boston (USA), July, 2002.

23. **Yong-Hyun Kim**, In-Ho Lee, and K.J. Chang, *Finite-temperature action-derived molecular dynamics simulations of the coalescence of C_{60} molecules*, The 26th International Conference on the Physics of Semiconductors, Edinburgh (UK), July, 2002.

24. J. Choi, **Yong-Hyun Kim**, K.J. Chang, and D. Tomanek, *Occurrence of itinerant ferromagnetism in C/BN superlattice nanotubes*, 5th Asian Workshop on First-Principles Electronic Structure Calculations, Seoul (Korea), October, 2002.

25. **Yong-Hyun Kim**, *Computational study of carbon nanostructures*, NREL Workshop on Computational Science in Material Science, Chemistry and Biology 2003 (NCS 2003), Golden (USA), April, 2003.

REFERENCES

Dr. Shengbai Zhang
National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, Colorado 80401
U.S.A
email) szhang@nrel.gov
tel) +1-303-384-6622
fax) +1-303-384-6655

Prof. Kee Joo Chang
Department of Physics
Korea Advanced Institute of Science and Technology
373-1 Kusung-Dong
Yusung-Gu, Daejeon 305-701
Korea

email) kchang@mail.kaist.ac.kr
tel) +82-42-869-2531
fax) +82-42-869-2510

Prof. David Tomanek
Department of Physics and Astronomy
Michigan State University
East Lansing, Michigan 48824-1116
email) tomanek@pa.msu.edu
tel) (517) 355-9702
fax) (517) 353-4500

Prof. Kang-Hun Ahn
School of Physics
Seoul National University
Seoul 151-742, Korea
email) khahn@phya.snu.ac.kr
tel) +82-2-880-5726

Prof. Dojun Youm
Department of Physics
Korea Advanced Institute of Science and Technology
373-1 Kusung-Dong
Yusung-Gu, Daejeon 305-701
Korea
email) djyoum@sorak.kaist.ac.kr
tel) +82-42-869-2530
fax) +82-42-869-2510