KYEONGJAE CHO, Ph.D.
Assistant Professor at Department of Mechanical Engineering
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RESEARCH AND TEACHING AREA

Multiscale modeling and simulation of nanomaterials. Modeling methods include atomistic and quantum simulations. structure-property relationships of nanoparticles, nanowires, and nanoscale interfaces are the main focus of modeling research. Research topics include metal nanoparticles, carbon nanotubes, semiconductor nanowires, and high-k gate stack interface problems. Main applications areas are device materials and clean energy technology. MSL simulator at NonoHUB (www.nanohub.org) illustrates the nanomaterial design concepts.

INDUSTRIAL APPLICATIONS OF ACADEMIC RESEARCH

Rational Design of Nanomaterials. The multiscale modeling software for nanomaterials was licensed by a start-up company (Nanostellar Inc.), and the company has integrated the modeling tool within a rational design and fabrication of catalyst nanomaterials to develop Pt replacement nanocatalyst for automobile catalytic converters. The multiscale modeling framework developed in my group is applied to Pt group metal nanoparticles to rationally design and optimize them for improved pollution control capacity.

EDUCATION

- Seoul National University, B.Sc. in Physics (1986)
- Seoul National University, M.Sc. in Physics (1988); Thesis entitled "**Studies on the Interference Effect between XPS and Auger Process**"
- Massachusetts Institute of Technology, Ph.D. in Physics (1994); Thesis entitled "**New Methods for Calculation of Dynamical Properties of Many-Particle Systems**"

POSITIONS

1994 - 1995	Postdoctoral Associate, Department of Physics, M.I.T.
1995 - 1996	Research Associate, Division of Engineering and Applied Sciences, Harvard University
1995 - 1997	Research Scientist, Research Laboratory of Electronics, M.I.T.
1997 - Present	Assistant Professor, Department of Mechanical Engineering, Stanford University
1999 - 2004	Assistant Professor by Courtesy, Department of Materials Science and Engineering, Stanford University
2003 - Present	Founder and Consultant of Nanostellar Inc.

JOURNAL PUBLICATIONS (Attachment 1: Publication List)

- 47 Main Archival Journal Papers
- 19 Secondary Archival Journal Papers
- 10 Miscellaneous Archival Journal Papers
- 19 Conference Proceeding Papers

PATENTS

- 4 United States Patents awarded
- 2 United States Patent applications filed

INVIDTED TALKS (Attachment 2: List of Invited Talks)

- 51 invited talks at international conferences and workshops
- 49 invited department seminars and tutorial talks

ACADEMIC AVITITY RECORD (Attachment 3: Academic Activity Record)

- 11 PhD students supervised (6 completed and 5 expected to complete during 2006-7)
- Teaching 23 quarters at Stanford University (5 materials science courses developed)
- Awarded 20 research funds from federal and industrial funding agencies

PROFESSIONAL ACTIVITIES

- Members of American Physical Society, Material Research Society, IEEE, ASME
- Referees for Physical Review Letters, Physical Review A, B and E, Material Science and Engineering, International Journal of Solids and Structures, Journal of Biochemistry, and Computational Materials Science
- Symposium Organizers/Chairs for MRS 99 Fall Meeting, USNCCM 99 Meeting, NSF Nanomechanics Workshop, ICES 2000 Meeting, MRS 2000 Fall Meeting, WCCM 2002 Meeting
- Members of Editorial Boards of Modeling and Simulation in Materials Science and Engineering (2001-2005), Computer Modeling in Engineering & Science (2002-present), and Journal of Computational and Theoretical Nanoscience (2003-present).
- Member of Stanford Materials Council (2000-2004) and Director of Stanford Computational Materials Science Lab (2001-2004)
- Technical Chair of Nanotechnology Committee in the U.S. Association of Computational Mechanics (2001 – 2003)

AWARDS/HONORS/OTHERS

- Sammi Industrial Fellowship (1985-1986)
- Moojin Science Foundation Fellowship (1988)
- Korean Government Overseas Study Fellowship (1988-1990)
- MIT Industry Liaison Fellowship (1988)
- Korean Government Overseas Graduate Student Award (1991)
- Korean Government Overseas Graduate Student Award (1992)
- "Simulating Reality" from PhD research work cited by White House Report on National Science Policy (Aug. 1994)
- Outstanding Young Researcher Awards, The Association of Korean Physicists in America (1996)
- Packard Foundation Frederich E. Terman Junior Faculty Fellowship (1997-2000)
- Veridian Outstanding Technical Authors Award (2000)
- Member of Technical Advisory Board, Profit Logic Inc. (2000 – 2003)
- Fellow of the Institute of Physics (2002-present)
- "Nanomaterials for Clean Energy," cited in President's Council of Advisors On Science And Technology Report **(**May 16, 2005).

REFERENCES

- **Robert W. Dutton**, Robert and Barbara Kleist Professor of Engineering
  Department of Electrical Engineering , Stanford University
  Office phone: 650-723-4138
  Email: dutton@gloworm.Stanford.EDU

- **John D. Joannopoulos**, Francis Wright Davis Professor of Physics
  Department of Physics, MIT
  Office phone: (617) 253-4806
  Email: joannop@MIT.EDU

- **William D. Nix**, Lee Otterson Professor of Engineering (Emeritus)
  Department of Materials Science and Engineering, Stanford University
  Office phone: 650-725-2605
  Email: nix@stanford.edu

- **Dr. Meyya Meyyappan**
  Director of Center for Nanotechnology, NASA Ames Research Center
  Office phone: (650) 604-2616
  Email: meyya@orbit.arc.nasa.gov

- **William F. Miller**, Herbert Hoover Professor of Management (Emeritus)
  Graduate School of Business, Stanford University
  Founder and Chairman of Nanostellar Inc.
  Office phone: (650) 723-3219
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Attachment 1: Publication List

JOURNAL PUBLICATIONS

- 47 Main Archival Journal Papers
- 19 Secondary Archival Journal Papers
- 10 Miscellaneous Archival Journal Papers
- 19 Conference Proceeding Papers

PATENTS: 4 United States Patents awarded, and 2 patent applications are filed.

Main Journal Publications

- Journal papers from graduate research and postdoctoral research are supervised by Prof. Oh (Seoul National University), Prof. J.D. Joannopoulos (MIT), and Prof. E. Kaxiras (Harvard).
- Journal papers from Stanford are research works of graduate students and postdoctoral associates I have supervised during 1997-2005.

Master Research at Seoul National University (1986 - 1988)

1. K. Cho and S.-J. Oh, "M4,5N4,5X Auger lineshapes of La compounds from one-step model calculations," Phys. Rev. B 39, 9576-9579 (1989).

PhD Research at MIT (1988 - 1994)

2. K. Cho and J. D. Joannopoulos, "**Ergodicity and dynamical properties of constant-temperature molecular dynamics**," Phys. Rev. A 45, 7089-7097 (1992).
3. K. Cho, J. D. Joannopoulos, and Leonard Kleinman, "**Constant-Temperature molecular dynamics with momentum conservation**," Phys. Rev. E 47, 3145-3151 (1993).
4. K. Cho and J. D. Joannopoulos, "**Tip-Surface Interactions in Scanning Tunneling Microscopy**," Phys. Rev. Lett. 71, 1387-1390 (1993).
5. K. Cho, T. A. Arias, J. D. Joannopoulos, and P. K. Lam, "**Wavelets in Electronic Structure Calculations**," Phys. Rev. Lett. 71, 1808-1811 (1993).
6. K. Cho and J. D. Joannopoulos, "**Tip-induced Modifications in Scanning Tunneling Microscopy and Atomic Force Microscopy**," Scanning Microscopy 9, 381-386 (1995).
7. K. Cho and J. D. Joannopoulos, "**Mechanical hysteresis on an atomic scale**," Surf. Sci. 328, 320-324 (1995).
8. K. Cho and J. D. Joannopoulos, "**Flipping silicon dimers on Si(100) using scanning tip microscopy: a theoretical investigation**," Phys. Rev. B 53, 4553-4556 (1996).
9. K. Cho and J. D. Joannopoulos, "**Reversible Tip-induced Structural Modifications in Scanning Tip Microscopy**," Jpn. J. Appl. Phys. 35, 3714-3718 (1996).

Postdoctoral Research at MIT & Harvard (1994 - 1997)

10. H. Lim, K. Cho, I. Park, J. D. Joannopoulos, and E. Kaxiras, "**Ab initio study of hydrogen adsorption on the Si(111)-(7x7) surface**," Phys. Rev. B 52, 17231-17237 (1995).
11. K. Cho, J. D. Joannopoulos, and A. N. Berker, "**Vicinal Si(100) surfaces under External Strain**," Phys. Rev. B 53, 1002-1005 (1996).
12. H. Lim, K. Cho, R. B. Capaz, J. D. Joannopoulos, K. D. Brommer, and B. E. Larson, "**Ab initio studies of adatom vacancies on the Si(111)-(7x7) surface**," Phys. Rev. B 53, 15421-15424 (1996).
13. K. Cho, E. Kaxiras, and J.D. Joannopoulos, "**Theory of adsorption and desorption of H2 molecules on the Si(111)-(7x7) surface**," Phys. Rev. Lett. 79, 5078 (1997).
14. K. Cho and E. Kaxiras, "**Intermittent Diffusion on the reconstructed Si(111) Surface**," Europhys. Lett. 39, 287 (1997).
15. K. Cho and E. Kaxiras, "**Ab initio study of metal adatom diffusion on the reconstructed Si(111) surface**," Surf. Sci. Lett. 396, L261 (1998).

Attachment 1: Publication List

Research at Stanford (1997 – 2005; names in **Bold – Graduate students,** *Italic – Postdocs***)**

16. S. Han, K. Cho, and J. Ihm, "**Ab initio study on the molecular recognition by metalloporphyrins: CO interaction with iron porphyrin**," Phys. Rev. E 59, 2218 (1999).
17. S. Han, K. Cho, and J. Ihm, "**Wavelets in All-Electron Density Functional Calculations**," Phys. Rev. B 60, 1437 (1999).
18. **A. Kawamoto**, **J. Jameson**, K. Cho, and R. Dutton, "**Challenges for Atomic Scale Modeling in Alternative Gate Stack Engineering**," IEEE Trans. Electron Dev. V.47, 1787 (2000).
19. **S. Peng** and K. Cho, "**Chemical Control of Nanotube Electronics**," Nanotechnology 11, 57 (2000).
20. **A. Kawamoto**, **J. Jameson,** P. Griffin, K. Cho, and R. Dutton, "**First-Principles Study of Hf and Zr Silicates for High-K Gate Dielectric Applications**," IEEE Electron Dev. Lett. 22, 14 (2001).
21. **A. Kawamoto**, K. Cho, and R. Dutton, "**First Principles Modeling of High-K Gate Dielectics**," J. Comp.-Aided Mat. Design v.8, no.1, p.39-57 (2001).
22. **A. Kawamoto**, K. Cho, P. Griffin, and R. Dutton, "**First Principles Investigation of Scaling Trends of Zirconium Silicate Interface Band Offsets**," J. Appl. Phys. 90, 1333 (2001).
23. **S. Park**, D. Srivastava, and K. Cho, "**Local reactivity of fullerenes and nano device design**," Nanotechnology 12, 245 (2001).
24. **S. Park,** D. Srivastava, and K. Cho, "**Model Qubits for Solid-State Quantum Computers: Endo-fullerene and Doped Diamond Nanocrystallite**," J. Nanoscience and Nanotechnology 1, 75 (2001).
25. **S. Peng** and K. Cho, "**Nano Electro Mechanics of Semiconducting Carbon Nanotube**," J. Appl. Mech. v.69, no.4, p.451-453 (2002).
26. **M. Haverty**, **A. Kawamoto**, K. Cho, and R. Dutton, "**First Principles Modeling of Aluminate High-k Gate Dielectric Materials**," Appl. Phys. Lett. 80, 2669 (2002)
27. K. Cho, "**First Principles Modeling of High-K Gate Dielectric Materials**," Computational Materials Science v.23, no.1-4, p.43-47 (2002).
28. **J. O'Keeffe**, *C. Wei*, and K. Cho, "**Band-structure modulation for carbon nanotubes in a uniform electric field**," Appl. Phys. Lett. 80, 676-678 (2002).
29. *C. Wei*, D. Srivastava, and K. Cho, "**Molecular dynamics study of temperature dependent plastic collapse of carbon nanotubes under axial compression**," Comp. Modeling in Engr. & Sci. 3, 255 (2002).
30. *M.I. Larsson, R.F. Sabiryanov*, K. Cho, B.M. Clemens, "**Nanopatterning of periodically strained surfaces: Predictive kinetic Monte Carlo simulation study**," J. Appl. Phys. v.94, no.5, p.3470-3484 (2003).
31. **P. Ramanarayanan**, K. Cho, B.M. Clemens, "**Effect of composition on vacancy mediated diffusion in random binary alloys: First principles study of the $Si_{1-x}Ge_x$ system**," J. Appl. Phys. v.94, no.1, p.174-185 (2003).
32. **A. Nojeh**, **G.W. Lakatos, S. Peng**, K. Cho, and R.F.W. Pease, "**A Carbon Nanotube Cross Structure as a Nanoscale Quantum Device**," Nano Lett. v.3, no.9, p.1187-1190 (2003).
33. **S. Park**, D. Srivastava, and K. Cho, "**Generalized Chemical Reactivity of Curved Surfaces: Carbon Nanotubes**," Nano Lett. v.3, no.9, p.1273-1277 (2003).
34. *C. Wei*, K. Cho, and D. Srivastava, "**Tensile yielding of multiwall carbon nanotubes**," Appl. Phys. Lett. v.82, no.15, p.2512-2514 (2003).
35. *M.I. Larsson, R.F. Sabiryanov*, K. Cho, and B.M. Clemens, "**Surface strain effects on adatom kinetics and self-assembly**," Surf. Sci. v.536, no.1-3, p.L389-L395 (2003).
36. **S. Peng** and K.Cho, "**Ab Initio Study of Doped Carbon Nanotube Sensors**," Nano Lett. 3(4), 513-517 (2003).

37. *R.F. Sabiryanov*, *M. I. Larsson*, K. Cho, W. D. Nix, and B. M. Clemens, "**Surface diffusion and growth of patterned nanostructures on strained surfaces**," Phys. Rev. B 67, 125412 (2003).
38. *C.Y. Wei*, K. Cho, and D. Srivastava, "**Tensile strength of carbon nanotubes under realistic temperature and strain rate**," Phys. Rev. B, v.67, no.11, p.115407-5407 (2003).
39. **S. Peng**, K. Cho, P. Qi, and H. Dai, "**Ab initio Study of CNT NO_2 gas sensor**," Chem. Phys. Lett. V.387 p.271-276 (2004).
40. *M.I. Larsson*, K. Cho, and B. Clemens, "**Surface diffusion mechanisms for strain-induced self-assembly**," Phys. Rev. B 69, p155426 (2004).
41. **P. Ramanarayanan**, B. Srinivasan, K. Cho, and B.M. Clemens, "**Migration energy for impurity diffusion in solids: A closer look**," J. Appl. Phys. 96, 7095 (2004).
42. **B. Shan** and K. Cho, "**Schottky Barrier at Metal/Nanotube Contact**," Phys. Rev. B 70, 233405 (2004).
43. **H.J. Liu** and K. Cho, "**A molecular dynamics study of round and flattened carbon nanotube structures**," Appl. Phys. Lett. 85, 807 (2004).
44. *S. Park*, L. Colombo, Y. Nishi, and K. Cho, "**Ab initio Study of Metal Gate Electrode Work Function**," Appl. Phys. Lett. 86, 73118 (2005).
45. **B. Shan** and K. Cho, "**First Principles Study of Work Functions of Single Wall Carbon Nanotubes**," Phys. Rev. Lett. **94,** 236602 (2005).
46. **B. Shan, G. Lakatos, S. Peng** and K. Cho, "**First Principles Study of band-gap change in deformed nanotubes**," Appl. Phys. Lett. 87, 173109 (2005).
47. **B. Shan** and K. Cho, "**First Principles Study of Work Functions of Double Wall Carbon Nanotubes**," Phys. Rev. B **73**, 081401(R) (2006).

Secondary Journal Publications

- Journal papers published in collaboration with other graduate students or postdocs during PhD and postdoctoral research.
- Journal papers from helping other research groups and collaborators in which I have played the secondary role of helping the research progress.

1. A. Devenyi, K. Cho, T. A. Arias, and J. D. Joannopoulos, "**Adaptive Riemannian metric for all-electron calculations**," Phys. Rev. B 49, 13373-13376 (1994).
2. R.B. Capaz, K. Cho, and J. D. Joannopoulos, "**Signatures of Bulk and Surface Arsenic Antisite Defects in GaAs(110)**," Phys. Rev. Lett. 75, 1811-1814 (1995).
3. S. Lee, S. J. Lee, J. Y. Lee, J. Kim, K. S. Kim, I. Park, K. Cho, J. D. Joannopoulos, "**Ab initio Study of Water Hexamer Anions**," Chem. Phys. Lett. 254, 128- 134 (1996).
4. K.S. Kim, I. Park, S. Lee, K. Cho, J. Y. Lee, J. Kim, J, D. Joannopoulos, "**The nature of a wet electron**," Phys. Rev. Lett. 76, 956-959 (1996).
5. J.W. Woo, R. C. Forrey, and K. Cho, "**Astrophysical EXAFS Tool**," Astrophysical Journal 477, 235-240 (1997).
6. R.C. Forrey, J. W. Woo and K. Cho, "**Astrophysical X-ray Absorption Near-Edge Structure Analysis**," Astrophysical Journal 505, 236 (1998).
7. S. Mirbt, N. Moll, K. Cho, and J.D. Joannopoulos, "**Novel Cation-Rich (100) Surface Reconstructions on InP and GaP**," Phys. Rev. B 60, 13283 (1999).
8. D. Srivastava, M. Menon, and K. Cho, "**Novel Nanoplasticity of Single-Wall Carbon Nanotubes under Uniaxial Compression**," Phys. Rev. Lett. 83, 2973 (1999).
9. J. Kong, N. Franklin, C. Zhou, M.G. Chapline, **S. Peng,** K. Cho, H. Dai, "**Nanotube Molecular Wires As Chemical Sensors**," Science v.287, 622 (2000).
10. D. Srivastava, M. Menon, and K. Cho, "**Anisotropic Nanomechanics of Boron Nitride Nanotubes: Nanostructures Skin Effect**," Phys. Rev. B 63, 195413 (2001).

11. I. Park, K. Cho, S. Lee, K.S. Kim, and J.D. Joannopoulos, "**Ab initio – Atomistic Dynamical Study of an Excess Electron in Water**," Comp. Mat. Sci. 21, 291 (2001).
12. D. Srivastava, M. Menon, and K. Cho, "**Computational Nanotechnology with Carbon Nanotubes and Fullerenes**," Computing in Science & Engineering 3, 42 (July/August 2001).
13. *C. Wei*, D. Srivastava, and K. Cho, "**Thermal Expansion and Diffusion Coefficients of Carbon Nanotube-Polymer Composites**," Nano Lett. 2(6), 647-650 (2002).
14. N.M. Ghoniem and K. Cho, "**The Emerging Role of Multiscale Modeling in Nano- and Micro-mechanics of Materials**," Comp. Modeling in Engr. & Sci. 3, 147 (2002).
15. D. Srivastava, *C. Wei*, and K. Cho, "**Computational Nanomechanics of Carbon Nanotubes and Composites**," Appl. Mech. Rev., 56:2, 215-230 (2003).
16. P. Qi, O. Vermesh, M. Grecu, A. Javey, Q. Wang, H. Dai, **S. Peng,** K. Cho, "**Toward Large Arrays of Multiplex Functionalized Carbon Nanotube Sensors for Highly Sensitive and Selective Molecular Detection**," Nano Lett;3(3); 347-351 (2003).
17. Y.M. Li, *S. Peng*, D. Mann, J. Cao, R. Tu, K. Cho, H. Dai, "**On the origin of preferential growth of semiconducting single-walled carbon nanotubes**," Journal of Physical Chemistry B v.109, no.15, p.6968-6971 (2005).
18. A. Nikitin, H. Ogasawara, D. Mann, R. Denecke, *Z. Zhang*, H. Dai, K. Cho, A. Nilsson, "**Hydrogenation of single-walled carbon nanotubes**," Phys. Rev. Lett. 95 (no.22), p.225507/1-4 (2005).
19. **A. Nojeh, B. Shan**, K. Cho, and R. F.W. Pease, "***Ab Initio* Modeling of the Interaction of Electron Beams and Single-Walled Carbon Nanotubes**," Phys. Rev. Lett. 96, 056802 (2006).

Miscellaneous Journal Publications

- Journal papers in which I have made minimal contributions.

1. P.D. Tepesch, A. F. Kohan, G. D. Garbulsky, G. Ceder, C. Coley, H. T. Stokes, L. L. Boyer, M. J. Mehl, B. P. Burton, K. Cho, and J. D. Joannopoulos, "**A Model to compute Phase Diagrams in Oxides with Empirical or First-principles Energy Methods and Application to the Solubility Limits in the CaO-MgO system**," J. Am. Ceram. Soc. 79, 2033-2040 (1996).
2. M.K. Aydinol, A. F. Kohan, G. Ceder, K. Cho and J. D. Joannopoulos, "**Ab initio Study of Lithium Intercalation in Metal-Dichalcogenides**," Phys. Rev. B 56, 1354 (1997).
3. J. Ireta, M. Galvan, K. Cho and J. D. Joannopoulos, "**Local Reactivity of Charybdotoxin a K+ Channel Blocker**," J. Am. Chem. Soc. 128, 9771 (1998).
4. R. Capaz, L.V.C. Assali, L.C. Kimerling, K. Cho, and J.D. Joannopoulos, "**A New Mechanism for Hydrogen-Enhanced Oxygen Diffusion in Silicon**," Phys. Rev. B 59, 4898 (1999).
5. T. Wang, N. Moll, K. Cho, and J.D. Joannopoulos, "**Deliberately Designed Materials for Optoelectronics Applications**," Phys. Rev. Lett. 82, 3304 (1999).
6. T. Wang, N. Moll, K. Cho, and J. D. Joannopoulos, "**Computational design of compounds for monolithic integration in optoelectronics**," Phys. Rev. B 63, 35306 (2000).
7. H. Zeng, *R. Sabibianov*, O. Mryasov, M.L. Yan, K. Cho, and D.J. Sellmyer, "**Curie Temperature of FePt: B_2O_3 Nanocomposite Films**," Phys. Rev. B v.6618, no.18, p.4425-4425 (2002).
8. Z.-R. Liu, H. Gao, L.Q. Chen, K. Cho, "**Patterned nanostructure in AgCo/Pt/MgO(001) thin films**," Phys. Rev. B v.68, no.3, p.035429 (2003).
9. J. Miller, K. Cho, M. McGehee, "**A realistic Assessment of the Commercialization of Nanotechnology: A Primer for Lawyers and Investors**," Nanotech Law & Business V.1, p1 (2004).

10. G.M. Rignanese, X. Gonxe, **G. Jun**, K. Cho, A. Pasquarello, "**First-principles investigation of high-k dielectrics: Compariosn between the silicates and oxides of hafnium and zirconium**," Phys. Rev. B 69, p18431 (2004).

Conference Proceeding Papers

1. K. Cho and J. D. Joannopoulos, "**The Devilish World of Surfaces**," in Toward Teraflop Computing and New Grand Challenge Applications, Eds. R. K. Kalia and R. Vashishta, Nova Science Publishers, 3-12 (1995).
2. T.A. Arias, K. Cho, J. D. Joannopoulos, P. K. Lam, and M. P. Teter, "**Wavelet- Transform Representation of the Electronic Structure of Materials**," in Toward Teraflop Computing and New Grand Challenge Applications, Eds. R. K. Kalia and R. Vashishta, Nova Science Publishers, 25-36 (1995).
3. K. Cho and E. Kaxiras, "**First-Principles Study of Si(111) Homoepitaxy**," MRS 98 Fall Meeting Proceedings 538, 341 (1999).
4. **A. Kawamoto**, J. Jameson, K. Cho, and R. Dutton, "**First Principles Investigation of Bulk Zirconium/Hafnium Silicate Materials for Alternative Gate Dielectric Applications**," SRC 2000 Techcon Conference Proceedings (2000).
5. **J.A. O'Keeffe**, N. Mingo, M.P. Anantram, and K. Cho, "**Band Structure Simulation of a Metal-Nanotube Junction**," SRC 2000 Techcon Conference Proceedings (2000).
6. **M. Haverty, A. Kawamoto, G. Jun,** K. Cho, and R. Dutton, "**Preliminary First-Principles Study of Hf and Zr Aluminates as Replacement High-k Dielectrics**," MRS 2001 Conference Proceeding (2001).
7. **S. Park**, D. Srivastava, and K. Cho, "**External Chemical Reactivity of Fullerenes and Nanotubes**," MRS 2001 Conference Proceeding Vol. 675, W1.5 (2001).
8. **S. Park**, D. Srivastava, and K. Cho, "**Endo-Fullerenes and Doped Bucky Onions as Seed Materials for Solid State Quantum Computers**," MRS Symposium Proceedings Vol. 675, W1.8 (2001).
9. **S. Peng** and K. Cho, "**Ab initio Study of Metal Atoms on SWNT Surface**," MRS 2001 Conference Proceeding Vo. 675, W4.8 (2001).
10. *C. Wei*, K. Cho, and D. Srivastava, "**Chemical Bonding of Polymer on Carbon Nanotube**," MRS 2001 Conference Proceeding Vol. 675, W4.7 (2001).
11. *C. Wei*, K. Cho, and D. Srivastava, "**Temperature and Strain-rate dependent Plastic Deformation of Carbon Nanotube**," MRS 2001 Conference Proceeding Vol. 677, AA6.5 (2001).
12. **S. Peng, J. O'Keeffe**, *C. Wei*, K. Cho, J. Kong, R. Chen, N. Franklin, H. Dai, "**Carbon Nanotube Chemical and Mechanical Sensors**," International Workshop on Structural Health Monitoring, 1142 (2001).
13. **G. Jun** and K. Cho "**First Principles Modeling Of High-K Dielectric Materials**," MRS 2002 Fall Meeting Conference Proceeding (2002).
14. K. Cho, **G. Jun, I. Choi, M. Haverty, A. Kawamoto,** and R. Dutton, "**First Principles Modeling of High-k Gate Dielectrics**," International Workshop on Device Technology, MRS Workshop Series (2002).
15. K. Cho, **G. Jun, I. Choi**, and R. Dutton "**First Principles Study of High-k Dielectric-Silicon Interfaces**," Proceedings of Third International Conference on Microelectronics and Interfaces, p.123 (2002).
16. *M.I. Larsson*, **B. Lee**, *R. Sabirynov*, K. Cho, W. Nix, and B.M. Clemens, "**Kinetic Monte Carlo Simulations of Strain-induced Nanopatterning on Hexagonal Surfaces**," MRS 2002 Spring Meeting Conference Proceeding (2002).
17. **B. Lee** and K. Cho, "**Atomistic Simulation Study of Controlled Nanostructure Patterning**," Material Research Society Proceedings 775 P.9.27 (2003).

18. *R.F. Sabiryanov*, K Cho, *MI Larsson*, WD Nix, BM Clemens, "**Growth and properties of small Co islands on a strained Pt surface**," J. Magnetism and Magnetic Materials v.258, p.365-368 (2003).
19. **P. Ramanarayanan**, *RF Sabiryanov*, and K Cho, "**Point defect energetics in silicon using the LDA+U method**," Transactions of the Materials Research Society of Japan 29 (8), p3625-3630 (2004).

PATENTS

1. K. Cho and J. D. Joannopoulos, "**Ultra High Density Memory Device**," United States Patent No. 5,448,514 (1995)
2. S. Onga, R.W. Dutton, K. Cho, H. Takada, and T. Okada, "**Semicondoctor Device Manufacturing Method**," United States Patent No. 6,514,885 (Feb. 4, 2003)
3. T. Wang, N. Moll, K. Cho, and J.D. Joannopoulos, "**Compound Semiconductor Structure with lattice and Polarity Matched heteroepitaxial Layers**," United States Patent No. 6,888,175 (May 3, 2005)
4. **J. O'Keeffe** and K. Cho, "**Band-Structure Modulation of Nano-Structure in an Electric Field**," United States Patent filed on Nov. 27, 2001 (Application No. 09/994,534).
5. K. Cho and **S. Peng**, "**Carbon Nanotube Sensors**," United States Patent filed on Jul. 11, 2002 and allowed on Oct. 13, 2005.
6. **B. Lee, S. Park,** and K. Cho, "**Nanoparticle Approach and Implementations therefor**," provisional United States Patent filed on Oct. 2004 by Stanford OTL.

Attachment 2: List of Invited Talks

INVIDTED TALKS

- 51 invited talks at International Conferences and Workshops
- 49 invited Department Seminars and tutorial talks

Invited Conference Talks:

1. "**Constant-temperature molecular dynamics**," *Telluride Summer Workshop,* (1991); Telluride, CO, USA.
2. "**STM tip-surface interactions**," *APS 1994 March Meeting,* (Mar. 21-25, 1994); Pittsburgh, PA, USA.
3. "**Tip-induced modifications in STM and AFM**," *Scanning Tunneling International,* (May 7-12, 1994); Toronto, Canada.
4. "**Wavelets in Electronic Structure Calculations**," *the 5th Italian-Swiss Workshop on Computational Condensed Matter Physics,* (Sep. 8-13, 1994); Sardinia, Italy.
5. "**First-principles study of semiconductor surfaces**," *Symposium on Parallel Computing: state of the art and applications,* (Oct. 27-28, 1994); Mexico City, Mexico.
6. "**Intrinsic Surface Atom Manipulations in STM and AFM**," *the 5th International Conference on the Formation of Semiconductor Interfaces,* (Jun. 26-30, 1995); Princeton, NJ, USA.
7. "**STM image of Si(100) surface**," ISPSA '94, (Oct. 15, 1994); Seoul, Korea.
8. "**Reversible tip-induced structural modifications in scanning tip microscopy**," *the 3rd International Colloquium on Scanning Tunneling Microscopy,* (Dec. 7-9, 1995); Kanazawa, Japan.
9. "**STM signature of the As antisite defect in GaAs**," *Gordon Research Conference on Point and Line Defects in Semiconductors,* (Aug. 18-23, 1996); Andover, NH, USA.
10. "**Density Functional Theory: from a wet electron to the concept of an ultra-high density memory device**," *1996 American Chemical Society Meeting,* (Aug. 25-29, 1996); Orlando, FL, USA.
11. "**Dynamical Processes on Silicon Surfaces**," *the 10th Workshop on Recent Developments in Electronic Structure Algorithms,* (May 29 – Jun. 1, 1998); U. Penn., Philadelphia, PA, USA.
12. "**Rare-Event Molecular Dynamics for Multiscale Mechanics**," *Symposium on Multiscale Analysis at the ASME Applied Mechanics & Materials Conference,* (Jun. 27-30, 1999); Blacksburg, VA, USA.
13. "**Stochastic Coupling between Atoms and Continuum**," *Symposium on Computational Methods for Multiscale Simulation of Materials at the 5th U.S. National Congress on Computational Mechanics,* (Aug. 4-6, 1999); Boulder, CO, USA.
14. "**Multiscale Simulations for Computational Nanomechanics**," *the 7th Foresight Conference on Molecular Nanotechnology,* (Oct. 15-17, 1999); Palo Alto, CA, USA.
15. "**Dynamical Processes on Semiconductor Surfaces**," *Symposium on Nanomechanics of Surfaces and Interfaces at Society of Engineering Science (SES) Meeting,* (Oct. 25-27, 1999); Austin, TX, USA.
16. "**Multiscale Modeling of Gate Dielectric Thin Films**," *Symposium on Multiscale Materials Modeling at IUMRS ICA 2000,* (Jul. 23-26, 2000); Hong Kong.
17. "**Computational Mechanics of Nanotubes**," *Symposium on Multiscale Simulations: Mechanics of Materials from Nano- to the Meso-scale at ICES2K,* (Aug. 23, 2000); Los Angeles, CA, USA.
18. "**Nanotube Mechanics**," *Symposium on Nanomechanics of surfaces and interfaces at ASME 2000,* (Nov. 10, 2000); Orlando, FL, USA.

Attachment 2: List of Invited Talks

19. "**Mechanics of Carbon Nanotubes**," *Mardi Gras Conference on Multiscale Simualtion, Theoretical, and Experimentla Approaches to Deformation, Friction, Fatigue and Fracture*, (Feb. 22-24, 2001); Baton Rouge, LA, USA. [*C. Wei*]
20. "**Nanotube Materials Mechanics**," *Symposium on Advances in Materials Theory and Modeling at MRS Spring Meeting*, (Apr. 16-20, 2001); San Francisco, CA, USA.
21. "**Accelerated Dynamics for Defect Evolution in Nanostructures**," *the 11th Lakeview Conference on Computational Research on Materials*, (May 9-11, 2001); Morgantown, WV, USA.
22. "**Time scale Problems in Atomistic Simulations**," *Computational Materials Science Network Workshop on Micro structural Effects on the Mechanics of Materials*, (Jun. 18-20, 2001); Berkeley, CA, USA.
23. "**Computational Nanotechnology: Nanotube Mechanics**," *Symposium on Modeling and Simulation of Micro and Nano Systems at the 6th U.S. National Congress on Computational Mechanics*, (Aug. 1-4, 2001); Dearborn, MI, USA.
24. "**First Principles Modeling of High-K Dielectric Materials**," *International Workshop on Device Technology*, (Sep. 3-5, 2001); Porto Alegre, Brazil.
25. "**Carbon Nanotube Chemical and Mechanical Sensors**," *the 3rd International Workshop on Structural Health Monitoring*, (Sep. 12-14, 2001); Stanford, CA, USA.
26. "**Accelerated Dynamics**," *International Workshop on Multiscale Modeling of Materials Strength and Failure*, (Oct. 7-9, 2001); Bodega Bay, CA, USA.
27. "**Nanotube Mechanics for Nanodevice Applications**," *Symposium on Nanoscale Materials and Structures at ASME 2001*, (Nov. 11-16, 2001); New York, NY, USA.
28. "**Chemical Reactivity Controlled Functionalization of Carbon Nanotubes**," *the 3rd Motorola Workshop on Computational Materials and Electronics*, (Nov. 12-14, 2001); Phoenix, AZ, USA. [**S. Park**]
29. "**First Principles Study of High-k Dielectric-Silicon Interfaces**," *the 3rd AVS International Conference on Microelectronics and Interfaces*, (Feb. 11-14, 2002); Santa Clara, CA, USA.
30. "**Multiscale Modeling of Patterned Nanostructures**," *International Symposium on Nano- and Micro-mechanics*, (June 17-20, 2002); London, UK.
31. "**Modeling of Nanostructure Patterning**," *the 14th U.S. National Congress of Theoretical and Applied Mechanics*, (June 23-28. 2002); Virginia Tech, Blacksburg, VA, USA.
32. "**Mechanically Controlled Functionalization of Carbon Nanotubes**," *2002 US-Korea Conference on Science, Technology and Entrepreneurship (UKC-2002)*, (July 8-13, 2002); Seoul, Korea. [**S. Park**]
33. "**Multiscale Modeling of Nanostructure Patterning**," *WCCM-V*, (Jul. 7-12, 2002); Vienna, Austria.
34. "**Ab initio Design of Nanotbe Chemical Sensors**," *Symposium on Nanotechnology & Nanosystem at ICES 2002*, (Jul. 31-Aug. 2, 2002); Reno, NV, USA. [**S. Peng**]
35. "**Quantum atomistic study of diffusion in silicon-germanium alloys**," *the 39th Annual Technical Meeting of the Society of Engineering Science (SES)*, (Oct. 13-16, 2002); Pennsylvania State University, PA, USA. [**P. Ram**]
36. "**Mechanics of Carbon Nanotubes and Device Applications**," *Symposium on Nanoscale Materials and Modeling at ASME*, (Nov. 19, 2002); New Orleans, LA, USA.
37. "**First Principles Modeling of High-K Dielectric Materials**," *MRS Fall Meeting*, (Dec. 4, 2002); Boston, MA, USA.

38. "**Ab initio Study of Metal Electrode Work function**," *International Workshop on Metal Gates/Workfunction Engineering*, (Aug 28-29, 2003); Stanford University, Stanford, CA, USA.
39. "**Multiscale Modeling for Nanosystem Design**," *ASME Integrated Nanosystems*, (Sep. 17-19, 2003); Palo Alto, CA, USA.
40. "**Hierarchical Multiscale Study of Metal Nanoparticles**," *SES Symposium on Atoms to Continua: Modeling Physics Hierarchically*, (Oct. 12-15, 2003); Ann Arbor, MI, USA. [**B. Lee**]
41. "**Carbon Nanotubes as Chemical Sensors**," *DOE-NSET Workshop on Artificially Structured Nanomaterials: Formation and Properties*, (Oct. 13, 2003); Gatllinburg, TN, USA. [**S. Peng**]
42. "**Describing point defects in silicon by extending the local density approximation with the Hubbard model**," *the 8th International Conference on Advanced Materials (ICAM) organized by the International Union of Materials Research Societies (IUMRS)*, (Oct. 8-13, 2003); Yokohama, Japan. [**P. Ram**]
43. "**Atomic scale study of high-k dielectric and metal gate electrodes**," *the 5th Motorola Workshop on Computational Materials and Electronics*, (Nov. 13-14, 2003); Austin, TX, USA.
44. "**Atomic Scale Studies of High-k Gate Dielectrics**," *MRS 2003 Fall Meeting*, (Dec. 1-5, 2003); Boston, MA, USA.
45. "**Multiscale Modeling of Nanosensors**," *the 3rd International Conference on Computational Modeling and Simulation of Materials*, (May 30-Jun. 4, 2004); Acireale, Italy. [**S. Peng**]
46. "**Mechanics of Nanotubes/Nanowires and Applications**," *International Workshop on Nanomechanics*, (Jul. 14 -17, 2004); Pacific Grove, CA, USA.
47. "**Multiscale Modeling for Nanosystem Design**," *2004 US-Korea Conference on Science, Technology and Entrepreneurship (UKC2004)*, (Aug. 12-14, 2004); Research Triangle Park, NC, USA.
48. "**Rational Design of Nanocatalyst**," *Clean Energy and Nanocatalyst Conference*, (Aug. 20, 2004); SRI, Menlo Park, CA, USA.
49. [Keynote talk] "**Nanosensor Design for Molecular Recognition**," *2004 SPIE Conference on Nanosensing: Materials and Devices*, (Oct. 25-28, 2004); Philadelphia, PA, USA.
50. "**Multiscale Modeling of Nanomaterials**," *Symposium on Materials by Design at ICCES 2005 Conference*, (Dec. 1-5, 2005); Chenni, India.
51. "**Multiscale Study of High-k Gate Stack**," the 53rd AVS Symposium (Nov. 12–17, 2006) San Francisco, CA, USA.

Invited Seminar Talks and Tutorials:

52. "**Ab initio Dynamics: Si(100) surface**," *Laboratory of Computer Science Seminar*, (Oct. 4, 1993); MIT, Cambridge, MA, USA.
53. "**First Principles Study of Semiconductor Surfaces**," *Chez Pierre Condensed Matter Physics Seminar*, (Sep. 9, 1994); MIT, Cambridge, MA, USA.
54. "**Ultra High Density Dimer Memory Device**," Samsung Electronics Co., (Oct. 17, 1994); Suwon, Korea.
55. "**First Principles Study of Semiconductor Surfaces**," *Physics Department Seminar*, (Oct. 18, 1994); Korea University, Seoul, Korea.

56. "**First Principles Study of Semiconductor Surfaces**," *Physics Department Seminar*, (Oct. 20, 1994); Kyung Hee University, Suwon, Korea.
57. "**First Principles Study of Semiconductor Surfaces**," *Physics Department Seminar*, (Dec. 13, 1995); Postech, Pohang, Korea.
58. "**First Principles Study of Point Defects on Semiconductor Surfaces**," *Physics Department Seminar*, (Dec. 14, 1995); KAIST, Korea.
59. "**Intrinsic Surface Atom Manipulation in STM and AFM**," *Physics Department Seminar*, (Dec. 16, 1995); Seoul National University, Seoul, Korea.
60. "**Electronic Structure Calculations at MIT Condensed Matter Theory Group**," *Gaussian Program Scientific Advisory Meeting*, (Apr. 20, 1996); New Haven, CT, USA.
61. "**Ab initio Study of Electronic Structures of Materials**," *Center for Astrophysics*, (Oct. 28, 1996); Harvard University, MA, USA.
62. "**First Principles Study of Epitaxial Growth on Semiconductor Surfaces**," *Physics Department Seminar*, (Jul. 11, 1996); Seoul National University, Seoul, Korea.
63. "**First Principles Study of Epitaxial Growth on Semiconductor Surfaces**," *Physics Department Seminar*, (Jul. 24, 1996); Yonsei University, Seoul, Korea.
64. "**Ab initio Prediction of Materials Behavior**," *Mechanical Engineering Department Seminar*, (Oct. 17, 1996); Stanford University, Stanford, CA, USA.
65. "**First Principles Study of Semiconductor Surfaces**," *Physics Department Seminar*, (Jan. 10, 1997); Boston University, Boston, MA, USA.
66. "**Microscopic Studies into the Behavior of Surfaces**," *Physics Department Seminar*, (Feb. 20, 1997); Philadelphia, PA, USA.
67. "**Theory of Adsorption and Desorption of H_2 on Si(111) surface**," *Physics Department Seminar*, (Jun. 10 1997); Seoul National University, Seoul, Korea.
68. "**Ab initio Study of Atoms and Molecules on Si(111) surface**," *Chemical Engineering Department Seminar*, (Oct. 29, 1997); Stanford University, Stanford, CA, USA.
69. "**Multiscale Simulations: Design Tool for Nanotechnology**," *Stanford Mechanics and Computation Division Seminar*, (Nov. 6, 1997); Stanford University, Stanford, CA, USA.
70. "**Ab initio Study of Scanning Tip Microscopy**," *Condensed Matter Physics Seminar*, (Jan. 11, 1998); Stanford University, Stanford, CA, USA.
71. "**Wavelets in Electronic Structure Calculations**," *SCCM Seminar*, (Jan. 26, 1998); Stanford University, Stanford, CA, USA.
72. "**Computational Nanomechanics: Mechanics and Electronics of Nanotubes**," *Stanford Mechanics and Computation Division Seminar*, (Oct. 14, 1999); Stanford University, Stanford, CA, USA.
73. "**Computational Nanomechanics: Mechanics and Electronics of Nanotubes and Balls**," *Stanford Materials Science & Engineering Colloquium*, (Nov. 12, 1999); Stanford University, Stanford, CA, USA.
74. "**Atomistic Modeling for Computational Nano Engineering**," *Stanford Center for Turbulence Research Seminar*, (Jan. 26, 2001); Stanford University, Stanford, CA, USA.
75. "**Computational Nano Engineering of Materials**," *Materials Group Seminar at Princeton University*, (Feb. 20, 2001); Princeton, NJ, USA.

76. "**First Principles Modeling of Materials**," *Tutorial Lecture at 2001 MRS Spring Meeting*, (Apr. 16-20, 2001); San Francisco, CA, USA.

77. "**Computational Nanotechnology: Nanotubes and Fullerenes**," *Stanford Nanotechnology Workshop,* (Jul. 19, 2001); Stanford University, Stanford, CA, USA.

78. "**Computational Nanotechnology: Nanotubes and Fullerenes**," *Smart Structure Research Center Workshop,* (Sep. 15, 2001); Sand Francisco, CA, USA.

79. "**Computer-Aided Design of Electronic Materials and Nanodevices**," *TCAD Group Seminar at Intel Corp.,* (Sep. 19, 2001); Santa Clara, CA, USA.

80. "**Computational Nanotechnology**," *Physics Department Colloquium at Virginia Polytech University*, (Oct. 26, 2001); VA, USA.

81. "**Computational Nanotechnology**," *Mechanical Engineering Department Colloquium at Northwestern University*, (Nov. 9, 2001); Evanston, IL, USA.

82. "**Research Projects at Stanford Multiscale Simulation Lab,**" *Multiscale Modeling, Simulation and Visualization Workshop*, (Mar. 5-6, 2002); NASA Langley Research Center, Hampton, VA, USA.

83. "**Multiscale Modeling of Nanostructure Patterning**," *ARO Workshop on Nanoscale Mechanics,* (Apr. 9-10, 2002); Panama City, FL, USA.

84. "**Multiscale Modeling for Nanomaterials Design**," *Mechanical Engineering Department Seminar at UIUC,* (Mar. 18, 2003); Urbana-Champagn, IL, USA.

85. "**Ab initio Study of Nanotube Sensors**," *North California Nano Teleconference*, (Jul. 16, 2003); Palo Alto, CA, USA.

86. "**Multiscale Modeling for Nanomaterials Design**," *the 2nd US-Korea Workshop on Nano-structured Materials and Nanomanufacturing,* (Aug. 9, 2003); Caltech, CA, USA.

87. "**Multi-Scale Computational Engineering of Nanotechnology**," *UKC 2003,* (Aug. 8-10, 2003); Caltech, CA. [**S. Park**]

88. "**Medical Applications of Nanotechnology**," *Kaiser Permanente Medical Center Grand Round*, (Aug. 13, 2003), South San Francisco, CA, USA.

89. [1/2 day tutorial] "**Computational Nanotechnology: Multiscale Modeling of Nanomaterials**," *Stanford Engineering and Science Institute: Nanoscience and Nanotechnology 2003,* (Aug. 18-22, 2003); Stanford, CA, USA.

90. [1/2 day tutorial] "**Multiscale Modeling for Nanostructure Patterning**," *UW-PNNL Nanoscience program,* (Sep. 19, 2003); University of Washington, Seattle, WA, USA.

91. "**Multiscale Modeling for Nanosystem Design**," *Mechanical Engineering Department Colloquium,* (Mar. 18, 2004); University of Missouri, Rolla, MS, USA.

92. "**Future Directions of Computational Mechanics Education**," *USACM Workshop on Computational Nanomechanics of Materials*, (Apr. 26-27, 2004); Chicago, IL, USA.

93. [1 day tutorial] "**Nanomaterials Modeling**," *Summer School on Computational Materials Science, Introduction to Computational Nanotechnology*, (Jun. 10, 2004); University of Illinois at Urbana-Champaign, IL, USA.

94. [1/2 day tutorial] "**Computational Nanotechnology: Multiscale Modeling of Nanomaterials**," *Stanford Engineering and Science Institute: Nanoscience and Nanotechnology,* (Jul. 27, 2004); Stanford, CA, USA.

Attachment 2: List of Invited Talks

95. [1/2 day tutorial] "**Advances in Computational Prototyping of Electronic Materials,**" *Stanford Engineering and Science Institute: New Electronic Materials for Extending Moore's Law*, (Aug. 26, 2004); Stanford, CA, USA.

96. "**Multiscale Modeling for Nanomaterials Design**," *Geophysics Department Seminar*, (Jan. 6, 2005); Stanford, CA, USA.

97. "**Is smaller stronger?**" *SMAC-Stanford Symposium*, (Apr. 18, 2005); Stanford, CA, USA.

98. "**Ab initio Study of Work Functions**," *Workshop on Metal Source/Drain Technology*, (May 12, 2005); Stanford, CA, USA.

99. "**Multiscale Modeling of Nanomaterials**," SKKU Advanced Institute of Nanotechnology, (Sep. 14, 2005); Sungkyunkwan University, Suwon, Korea.

100. "**Computational Nanotechnology and Nanomaterials Modeling**," KIAS Seminar, (Dec. 21 and 22, 2005); Seoul, Korea.

Attachment 3: Academic Activity Record

DOCTORAL STUDENTS SUPERVISED

Completed PhD Students

- Atshushi Kawamoto (1997 – 2001; PhD in EE Department, Stanford) [Co-Advisor]
  Thesis title: "**Atomic Scale Modeling of Silicate Interface Properties for High-*k* Gate Dielectric Applications"**
- Shu Peng (1997 – 2003; PhD in ME Department, Stanford)
  Thesis title: "**Simulation & Modeling of Carbon Nanotube Devices**"
- Seongjun Park (1997 – 2003; PhD in ChemE Department, Stanford)
  Thesis title: "**Multi-scale computational engineering of nanotechnology**"
- P. Ramanarayanan (1998 – 2004; PhD in ME Department, Stanford)
  Thesis title: "**Hierarchical Multiscale Modeling of Solid State Diffusion**"
- James O'Keeffe (1998 – 2004; PhD in EE Department, Stanford) [Co-Advisor]
  Thesis title: "**Transport in Nanotube Electronics and Organic Nanopores**"
- Byeongchan Lee (1999 – 2005; PhD in ME Department, Stanford)
  Thesis title: "**Multiscale Study of Metal Nanoparticles**"

Current PhD Students

- Ali Nojeh (2000 – 2006 expected; PhD in EE Department, Stanford) [Co-Advisor]
- Henry Liu (2001 – 2006 expected; PhD in ME Department, Stanford)
- Bin Shan (2001 – 2006 expected; PhD in Appl. Phys. Department, Stanford)
- Jeong-hee Ha (2002- 2007 expected; PhD in MSE Department, Stanford) [Co-Advisor]
- Paul Leu (2002- 2007 expected; PhD in ME Department, Stanford)

TEACHING EXPERIENCE

Main themes of course development

- Atomistic modeling and simulations using molecular dynamics (MD), Monte Carlo (MC), and kinetic Monte Carlo (kMC) methods
- Quantum modeling and simulations using tight-binding (TB) and density functional theory (DFT) methods
- Atomic structure, electronic structure, and dynamic properties of solid materials
- Applications to nanomaterials (nanoparticles and nanowires) modeling and analysis
- Design of solid materials and atomistic analysis

List of courses during 1998 - 2006

1. 1998 Winter Quarter: ME244 Atomistic Simulations of Materials
2. 1998 Spring Quarter: ME249 Quantum Nature of Materials
3. 1998 Autumn Quarter: ME229 Physical Solid Mechanics
4. 1999 Winter Quarter: ME244 Atomistic Simulations of Materials
5. 1999 Spring Quarter: ME238B Atomistic Analysis of Continuum Mechanics
6. 1999 Summer Quarter: ME390 Engineering Quantum Mechanics
7. 1999 Autumn Quarter: ME238A Continuum Mechanics
8. 2000 Winter Quarter: ME244 Atomistic Simulations of Materials
9. 2000 Spring Quarter: ME249 Quantum Nature of Materials
10. 2000 Autumn Quarter: ME238A Continuum Mechanics
11. 2001 Winter Quarter: ME238B Atomistic Analysis of Continuum Mechanics
12. 2001 Spring Quarter: ME229 Physical Solid Mechanics
13. 2001 Autumn Quarter: ME244A Computational Nanotechnology
14. 2002 Winter Quarter: ME244B Atomistic Simulations
15. 2002 Spring Quarter: ME249 Quantum Simulations
16. 2002 Autumn Quarter: ME344A Computational Nanotechnology
17. 2003 Autumn Quarter: ME344A Computational Nanotechnology
18. 2004 Winter Quarter: ME344B Nanomaterials Modeling
19. 2004 Spring Quarter: ME240 Introduction to Nanotechnology
20. 2004 Autumn Quarter: ME329 Physical Solid Mechanics
21. 2005 Winter Quarter: ME344A Computational Nanotechnology
22. 2005 Spring Quarter: ME344B Nanomaterials Modeling
23. 2006 Winter Quarter: ME344A Computational Nanotechnology
24. 2006 Spring Quarter: ME344B Nanomaterials Modeling (planned)

RESEARCH FUNDING (Source, Role, Period, Total fund, Title)

1. Packard Foundation, PI, 9/1/1997 - 8/31/2000, $275K, "**Multiscale Simulations**"
2. LLNL, PI, 2/3/1999 - 9/30/2001, $90K, "**Multiscale Simulation Tool Development: Accelerated Molecular Dynamics**"
3. DOE, Co-PI, 9/15/1999 - 9/14/2002, $80K/year, "**Coupled Interdiffusion and Misfit Stress Relaxation in Epitaxial Si/SiGe Heterostructures**"
4. SRC, Lead PI, 1/1/2000 - 12/31/2002, $100K/year, "**First Principles Modeling of High-K Gate Dielectrics**"
5. NSF, Co-PI, 9/1/2000 - 8/31/2003, $1,700K, "**Computational Nano-Engineering for Patterned Magnetic Nanostructures**"
6. Sandia National Lab, PI, 6/1/2000 - 9/30/2002, $120K, "**Multiscale Dynamics: Coupling Continuum to Atomistics**"
7. NASA, PI, 7/1/2001 - 5/31/2002, $43K, "**Simulation-Based Prototyping of Solid-State Quantum Computers**"
8. NASA, PI, 10/1/00 - 9/30/02, $125K, "**Simulation-based Design of Smart Nanotube Composite Materials**"
9. NSF-NIRT, Co-PI, 5/1/2002 - 4/30/2006, $90K/year, "**Properties and Applications of Deformed Nanotubes**"
10. NSF, Co-PI, 5/1/2002 - 4/30/2005, $80K/year, "**Reliability of Ferroelectric Thin Films: A Systematic Study of Point Defect Phenomena and Local Electronic Structure Effects**"
11. SRC, Co-PI, 8/1/2002 - 7/31/2005, $75K/year, "**Atomic Scale Studies of High-*k* Gate Dielectrics: Interfaces, Phase Changes and Dielectric Properties**"
12. NSF-CPIMA, Seed Project PI, 9/1/2002 – 8/31/2004, $100K, "**Molecular Recognition for Guided Self-Assembly of Polymers on Patterned Surfaces**"
13. MARCO-MSD, Co-PI, 9/1/2003 - 8/31/2006, $75K/year, "**Multiscale Modeling for Computational Nano-Engineering of Metal Alloys**"
14. Intel, PI, 11/1/2003 - 10/31/2006, $360K, "**Quantum transport Modeling of Nanostructure devices**"
15. GCEP, Lead PI, 1/1/04 - 12/31/06, $2,250K, "**Nanoengineering of Hybrid Carbon Nanotube – Metal Nanocluster Composite Materials for Hydrogen Storage**"
16. NSF-NCN, Co-PI, 8/1/2002 - 7/31/2007, $100K/year, "**Nanotube electronics**"
17. NSF-NSEC (UC Berkeley COINS), Co-PI, 9/1/2004 - 8/31/2009, $50K/year, "**Multiscale Modeling of Nanomaterials**"
18. NSF-NSEC (Stanford CPN). Co-PI, 9/1/2004 - 8/31/2009, $85K/year, "**Multiscale Modeling of Scanning Probes**"
19. NSF-NER, Co-PI, 9/1/2004 - 8/31/2005, $50K, "**Coordinated Multi-scale Simulations and *In situ* Electron Microscopy to Elucidate the Mechanisms of Nanowire Formations**"
20. Stanford CIS INMP, Co-PI, 5/1/2003 - present, $100K/year, "**Multiscale Modeling of High-K Gate Dielectric Materials**"