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PRESENT POSITION Physicist

EDUCATION Ph.D., Theoretical Solid State Physics, University of California, Davis, CA, 1989.

RESEARCH INTERESTS

Atomistic simulations of defect structures in bcc metals. Computer simulations of classical and quantum systems using molecular dynamics and quantum molecular dynamics methods. Electronic structures of surface and interface problems. Algorithm development on massively parallel processor platforms.

RESEARCH EXPERIENCES

- Nonlinear optimization by dynamical simulated annealing.
- Electron transport in materials using quantum molecular dynamics simulations
- Electronic properties of device materials, semiconductor superlattices, and metal-semiconductor interfaces.
- Large-scale *ab initio* calculations of transition metal surfaces, defects and dopants in semiconductors.

- Structural and thermodynamical properties of point defects in metals and alloys.
- Atomistic simulations of misfit-defect structures and solute segregation at ceramic/metal interfaces, including potential fittings from *ab initio* calculations.
- Atomistic simulations of dislocation process in bcc transition metals.
- Algorithm development for large-scale computer simulations on parallel architectures.
- Large-scale computing on massively parallel processor platform

PROFESSIONAL EXPERIENCES

Oct. (1988) - Jan. (1991), Postdoctoral Fellow, Argonne National Laboratory, IL.

Feb. (1991) - Jan. (1994), Postdoctoral Staff, Lawrence Livermore National Laboratory, CA.

Feb. (1994) – Present, Physicist, Lawrence Livermore National Laboratory, CA.

AFFILIATIONS, AWARDS and COMMITTEES

- The American Physical Society.
- The Materials Research Society.
- Served in a proposal review committee for Institute of Scientific Computing at Lawrence Livermore National Laboratory, 1994.
- Served in an independent peer review panel for research projects funded by DOE's Office of Energy Efficiency and Renewable Energy, 1994.

PUBLICATIONS:

1. The Doping Mechanism in Amorphous Silicon, C. S. Nichols, L. H. Yang, and C. Y. Fong, J. Non-Cryst. Sol. **97** & **98**, 495 (1987)
2. Localization of Multivibrational Excitations, M. S. Wartak, L. H. Yang, C. Y. Fong, and Y. R. Shen, Phys. Rev. B **37**, 10350 (1988).
3. Electronic Properties of Si-Ge Micro NIPI Structure, L. H. Yang, C. Y. Fong, and J. S. Nelson, " Heteroepitaxy on Silicon: Fundamentals, Structures, and Devices", eds H. K. Choi, R. Hull, H. Ishiwara, and R. J. Newmanich (MRS, Pittsburgh, 1988), p513.
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5. A Theoretical Study of Na Overlayers on the GaAs(110) Surface, C. Y. Fong, L. H. Yang, and Inder P. Batra," Metallization and Metal-Semiconductor Interfaces", ed. Inder P. Batra (Plenum, New York, 1989), p449.
6. Electronic Properties of Micro *n-i-p-i* Structures in Silicon Superlattices, L. H. Yang, R. F. Gallup, C. Y. Fong, and J. S. Nelson, Phys. Rev. B **39**, 3795 (1989)
7. Electronic Properties of Na Overlayers on the GaAs(110) Surface, C. Y. Fong, L. H. Yang, and Inder P. Batra, Phys. Rev. B **40**, 6120 (1989)
8. Electronic Properties of the Donor States Under Two-dimensional-conductor and Quantum-wire Configurations in Heavily and Orderly Doped (GaAs)-(AlAs), C. Y. Fong, L. H. Yang, J. S. Nelson, and L. Esaki, Phys. Rev. B**41**, 10667 (1990).
9. Compensated Dopants in Hydrogenated Amorphous Silicon, L. H. Yang and C. Y. Fong, "Amorphous Silicon Technology", eds Y. Hamakawa, P. G. LeComber, A. Madan, P. C. Taylor, and M. J. Thompson (MRS, Pittsburgh, 1989), Vol. 191, p445.
10. Quantum Molecular Dynamics - A New Algorithm for Linear and Nonlinear Electron Transport in Disordered Materials, R. K. Kalia, P. Vashishta, L. H. Yang, F. Dech, and J. Rowlan, The Inter. J. Supercom. App. **4**, 22 (1990).
11. Electron Trapping in Amorphous Silicon - A Quantum Molecular Dynamics Study, L. H. Yang, R.K. Kalia, and P. Vashishta, "Amorphous Silicon

Technology", eds Y. Hamakawa, P. G. LeComber, A. Madan, P. C. Taylor, and M. J. Thompson (MRS, Pittsburgh, 1990), Vol. 192, p781.

12. Impurity-Defect Complexes in Hydrogenated Amorphous Silicon, L. H. Yang, C. Y. Fong, and C. S. Nichols, "Amorphous Silicon Technology", eds Y. Hamakawa, P. G. LeComber, A. Madan, P. C. Taylor, and M. J. Thompson (MRS, Pittsburgh, 1991).

13. Impurity-Defect Complexes and Doping Mechanism in Hydrogenated Amorphous Silicon, L. H. Yang, C. Y. Fong, and C. S. Nichols, Phys. Rev. Lett. **66**, 3273 (1991).

14. Formation Energy and Lattice-Relaxation for Point Defects in Li and Al, R. Benedek, L.H.Yang, C. Woodward, and B.I. Min, Phys. Rev. B**45**, 2607 (1992).

15. Probing Excess Electron Localization and Mobility in Amorphous Silicon by Quantum Molecular Dynamics Method, A. Nakano, P. Vashishta, R. K. Kalia, and L. H. Yang, Phys. Rev. B**45**, 8363 (1992).

16. Possible Doping Mechanism in Hydrogenated Amorphous Silicon — an Impurity-Defect Complex Model, C. Y. Fong and L. H. Yang, Mod. Phys. Letts. B**6**, 235 (1992).

17. Polymeric Nitrogen, C. Mailhiot, L. H. Yang, and A. K. McMahan, Phys. Rev. B**46**, 14419 (1992-II).

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19. A Link-Cell Domain Decomposition Method for Molecular Dynamics Simulation on a Scalable Multiprocessor, L. H. Yang, E. D. Brooks III, and J. Belak, Scientific Programming **1**, 153 (1993).

20. Bonding Properties of the Interacting Donor and Acceptor States of Si-doped *n-i-p-i* Structures in GaAs, C. Y. Fong, J. S. Nelson, and L. H. Yang, Modeling and Simul.Mater. Sci. and Eng. **1**, 349 (1993).

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22. The Insulator-Metal Transition in Expanded Cesium, M. Ross, L. H. Yang, B. Dahling and N. Winter, Zeitschrift Für Physikalische Chemie, Bd. 184, S.65 (1994).

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26. Atomic Potentials for Rb- and K- Graphite Intercalation Compounds, R. Benedek, A. P. Smith, and L. H. Yang, Phys. Rev. B**49**, 5050 (1994).

27. Band Discontinuities at Heterojunctions between Crystalline and Amorphous Silicon, C.G. Van de Walle and L.H. Yang, J. Vac. Sci. & Tech. **B**13, 1635 (1995).

28. *Ab-initio* Pseudopotential Calculations of Point Defects and Boron Impurity in Silicon, J. Zhu, L.H. Yang, C. Mailhiot, T. Dias de la Rubia, and G. Gilmer , Nuclear Instruments and Methods in Physics Research, **B**102, 29 (1995).

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65. Reaction Path for Te During Surfactant-Mediated Epitaxial Growth of GaAs (100), C. D. Consorte, C. Y. Fong, M. D. Watson, L.H. Yang, and S. Ciraci, Phys. Rev. **B63**, 041301(**R**) (2001).

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