

## Curriculum Vitae

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## EDUCATION

- Ph. D. Ohio State University, Department of Physics, August 1996.  
Thesis advisor: Professor John W. Wilkins  
Coadvisor : Professor Furrukh S. Khan (EE)
- B.S. Korea Advanced Institute of Science and Technology (KAIST),  
Physics (magna cum laude), February 1991.

## PROFESSIONAL EMPLOYMENT

- 10/97 to present NSF-CISE Postdoctoral Fellow  
Supervisor: Prof. John W. Wilkins
- 9/96 to 8/97 Associated Western University (AWU) Postdoctoral Fellow, NREL  
Supervisor: Dr. Alex Zunger.
- 9-11/94, 10/95 Visiting researcher at IRRMA, Lausanne, Switzerland.  
Supervisor: Dr. Giulia Galli.
- 9/94 to 8/96 Research assistant, Department of Physics, Ohio State University.  
Supervisor: Professor John W. Wilkins.
- 9/92 to 8/94 Teaching assistant, Department of Physics, Ohio State University.  
Duties involved leading recitations for introductory physics courses.  
Supervisors: Dr. Richard Syler and Dr. Michelle Rallis.
- Summer 1993 Visiting researcher in the Condensed Matter Theory Group,  
Brookhaven National Laboratory.  
Supervisors: Dr. Furrukh Khan and Dr. James Davenport.
- 3/91 to 6/91 Research assistant, Space Science Lab (KAIST).  
Involved with the Space Plasma Project.  
Supervisor: Professor Kyung-wook Min.

## ACADEMIC HONORS

- |                                      |                                                 |
|--------------------------------------|-------------------------------------------------|
| Ohio State University (1997-present) | NSF-CISE Postdoctoral Fellowship (1997-present) |
| NREL (1996-1997)                     | AWU Postdoctoral Fellowship (1996-1997)         |
| Ohio State University (1991-1996)    | University Fellowship (1991-1992)               |
|                                      | Rotary International Fellowship (1992-1993)     |
| KAIST (1987-1991)                    | College Scholarship (1987-1991)                 |

## RESEARCH AWARDS

National Partnership for advanced computational infrastructure (NPACI), “dynamical simulations of large-scale defect structures in a tight-binding representations”, Mar/98 - Mar/99,

100000 SU on parallel computers (IBM SP2/Cray T3E/SGI O2000) at SDSC on NCSA; continued support Mar/99 - Mar/00.

## COMPUTER SKILLS

Languages: C/C++, Fortran, Fortran 90, Java

Machines: Unix workstations, Cray Y-MP8, SGI O2000, Cray T3D/E, IBM SP2

## LANGUAGE SKILLS

Korean (native); English (excellent); German (good)

## RESEARCH ACCOMPLISHMENT

Tight-binding molecular dynamics simulations on massively parallel computers: I developed a parallel algorithm for molecular dynamics (MD) simulations based on a tight-binding Hamiltonian for silicon in collaborations with M. Y. Yeh, F. S. Khan and J. W. Wilkins. A factor of 10 – 100 speed up is achieved by using the parallelized Car-Parrinello fictitious Lagrangian method. I performed MD simulations of bulk silicon and Si(111)- $7\times 7$  reconstructed surface. The vibrational spectrum is reproduced with a resolution of 0.1 THz. The localized phonons at adatomic sites, observed by EEL spectroscopy, are reproduced by MD simulations of the surface. We also observe a new highly symmetrical collective mode of the surface layer atoms.

Orbital-based linear scaling method: total energy global optimization using nonorthogonal localized orbitals: I proposed a new method to eliminate the local minima problem in the orbital-based  $O(N)$ -method by using larger set of nonorthogonal localized orbitals than occupied states and the electronic chemical potential in an energy functional. This work is done in collaborations with G. Galli and F. Mauri. The global minimum of the electronic structure is variationally obtained independent of the initial inputs of orbitals, while linear scaling with respect to the system size is maintained.

Ordered and disordered solid forms of  $C_{28}$ : I performed MD simulations of the growth of a disordered form of solid  $C_{28}$  (a- $C_{28}$ ) by sequences of low energy collisions of  $C_{28}$ 's with an  $O(N)$  tight-binding method. This work was done in collaborations with G. Galli, A. Canning, and J. W. Wilkins. I compare the physical properties of a- $C_{28}$  with those of the hyperdiamond structure, a proposed solid form of  $C_{28}$  considering four preferred active sites.

Extended defects in Si: I studied the equilibrium structure of large-scale defects produced in silicon by ion implantation by using orbital-based linear-scaling method in tight-binding representations. Experiments suggest that the  $\{311\}$ -defects provide sources and sinks of Si-interstitials which are believed to transiently enhance the diffusion of dopants. I find hierarchy of stability of interstitial defects exists – elongated interstitial clusters, interstitial chains and extended  $\{311\}$  defects. I proposed energetically favorable mechanisms which can lead to the displacement of interstitial chains and can explain the growth of the  $\{311\}$  defects and related structures such as V-shape bend structures and atomic steps observed in transmission electron microscopy images.

Electronic structures of GaAs/AlAs nanostructures: in collaboration with A. Zunger, I studied the quantum confinement of (i) multiple quantum wells of flat GaAs and AlAs layers, *i.e.*  $(\text{GaAs})_m/(\text{AlAs})_n/(\text{GaAs})_p/(\text{AlAs})_q$ , and (ii) “cylindrical Russian Dolls” – an equivalent sequence of wells and barriers arranged as concentric wires. A charge separation in

two GaAs wells is predicted in cylindrical Russian Doll structures for a particular choice of layer thicknesses. The origin of this charge separation is (i) *two-dimensional confinements* of charge carriers and (ii) heavy-hole anisotropy.

Empirical pseudopotentials of lattice mismatched III-V compounds: I developed empirical pseudopotentials to give correct descriptions of band structures under hydrostatic deformations as well as those at bulk equilibriums. New screened atomic pseudopotentials take account the strain effect explicitly and thus can be used for systems consisting of lattice mismatched materials, *e.g.*, InAs dots grown on GaAs substrates.

Elastic and optical properties of InAs dots: I studied the elastic and optical properties of pyramidal InAs dots grown on GaAs substrates by the Stranski-Krastanov (SK) growth mechanism. I find that the dot shape as well as the size have significant effect on its electronic structure due to the significant modification of the strains in the dot and in the barrier in the presence of large lattice mismatch. I relate several observable quantities, such as energy gaps and energies of excited electron and hole states, to the geometrical variables. These findings can be used to determine the physical shapes of the embedded dots.

Stability of interstitial defects in silicon: from point to extended defects I found trends in the formation energies of  $n$ -interstitial defects. Using first-principle calculations within the local density approximation (LDA), we consider relevant interstitial defects - small clusters ( $n=2-5$ ), chains, and planar  $\{311\}$  defects - and we relate them to growth of interstitial defects in interstitial supersaturated silicon as achieved in ion-implanted samples. In general, the stability of interstitial clusters increases as the size  $n$  increases. Preferred elongation of rod-like defects in the  $[011]$  direction is predicted in accordance with experiments. We find that the stable configuration for a given size can be (a) *compact* for small clusters, (b) *elongated* for medium clusters and (c) *planar* for large clusters.

## CURRENT RESEARCH\*

Development of object-oriented codes: I develop object-oriented codes using C++ to perform molecular dynamics simulations with atomistic potentials (classical/tight-binding/ first-principle). For a given system and the physical process of interest, the potential and efficient algorithms will be chosen based on (i) the accuracy required to describe important interactions (ii) the system size to take account interactions at different length scales, (iii) the time scale of the dynamical process. Different problems should be investigated with appropriate data structures and algorithms, while maximizing reuse of the code. This can be accomplished efficiently by developing code in object-oriented frameworks. The MD codes are built on POOMA (Parallel Object Oriented Methods and Applications) by LANL which provides underlying objects responsible for parallelism and node-level simulations for efficiency, portability and re-usability. This code is designed for educational use, as well as for researches in materials science. It provides simple and user-friendly interfaces and interactive visualizations that can greatly enhance understanding of microscopic physics for non-specialists.

Carbon-silicon defects: in collaborations with Thomas Fraueheim at University of Paderborn, Germany. Substitutional carbons trap interstitial silicon, thus reducing formation of interstitial defects that enhance boron diffusion. However, the presence of a high concentration of C and C-Si agglomerates can also deteriorate the device properties, *e.g.*, enhanced

\* Under supervision of Prof. John W. Wilkins

junction leakage. The clustering of carbon and silicon can significantly affect the electronic structure which conventional tight-binding schemes often fails to describe. By using self-consistent tight-binding Hamiltonians, we can study the materials containing multi species, while retaining the favorable computational cost to that of LDA calculations in dealing with the large systems necessary to describe C-Si agglomerates.

Electronic structures of point defects in Si: in collaborations with Dr. W. Aulbur and Dr. F. Kirchhoff, I study electronic structures of interstitials and di-interstitials in Si by density-functional quasiparticle calculations within GW approximations. Small interstitial clusters are building blocks of the  $\{311\}$  extended defects and play crucial roles in dopant diffusion during an implantation damage anneal. We have identified stable interstitial clusters consisting of  $\langle 110 \rangle$ -interstitialcy and found stable di-interstitial structures. Recently, Y. H. Lee at IBM [Appl. Phys. Lett. **73**, 1119 (1998)] suggested a model structure of a di-interstitial based on electron paramagnetic resonance (EPR) experiments, whose symmetry is in a good agreement with our structural models. We investigate the identity of defect states and the effect of uni- and bi-axial stress on the defect states following the EPR experiments. Dr. Lee proposed to look for other optical and vibration signatures unique to the di-interstitials.

Dynamics simulation of defected materials: I study thermal properties of the  $\{311\}$  extended defects by molecular dynamics simulations. In particular, I investigate the role of the extended defects in the interstitial diffusions to clarify the transient enhanced diffusion in ion-implanted silicon. Recently developed hyper-MD method [A. Voter, Phys. Rev. Lett. **78**, 3908 (1997); M. Steiner, M. M. Steiner, P.-A. Genilloud, and J. W. Wilkins, Phys. Rev. B **57**, 10236 (1998)] is being tested to perform time scale of 10 – 100 nsec, which has been beyond the scope of the conventional MD scheme. For classical potentials, we achieve boost factors of  $10^3$  by exploiting the locality of interactions. In collaborations with F. Kirchhoff and J. W. Wilkins, I study diffusion of point defects essential for understanding the mechanical properties of transition metal alloys at elevated temperatures. Titanium and its alloys are an important class of metallic materials which are used extensively in energy, aerospace and biomedical applications. Titanium alloys have very high specific strength (i.e., ratio of yield strength/density), good fracture toughness, and excellent corrosion resistance.

## PUBLICATIONS

- “Stability of Si-interstitial defects: from point to extended defects,” J. Kim, F. Kirchhoff, J. W. Wilkins, and F. S. Khan, Phys. Rev. Lett. **84**, 503 (2000).
- “Thermally activated reorientation of di-interstitial defects in silicon”, J. Kim, F. Kirchhoff, W. G. Aulbur, J. W. Wilkins, F. S. Khan and G. Kresse, Phys. Rev. Lett. **83**, 1990 (1999).
- “Electronic structures of  $[110]$  faceted “self-assembled” pyramidal InAs/GaAs quantum dots”, L. W. Wang, J. Kim and A. Zunger, Phys. Rev. B **59**, 5678 (1999).
- “Assembling small fullerenes: a molecular dynamics study”, G. Galli, A. Canning and J. Kim, to appear in ‘Covalently bonded disorder thin-film materials’, Eds. M. P. Siegal, J. E. Jaskie, W. Milne and D. McKenzie (1998).
- “Large scale quantum simulations using Tight-Binding Hamiltonians and linear scaling methods”, G. Galli, J. Kim, A. Canning and R. Haerle, ‘Tight-Binding Approach to Computational Materials Science’, Eds. P. Turchi, A. Gonis and L. Colombo, 425 (1998).

- “Comparison of the electronic structure of InAs/GaAs pyramidal quantum dots with different facet orientation”, J. Kim, L. W. Wang and A. Zunger, Phys. Rev. B **57**, R9408 (1998).
- “Comparison of two methods for describing the strain profiles in quantum dots”, C. Pryor, J. Kim, L. W. Wang, A. J. Williamson, and A. Zunger, J. App. Phys. **83**, 2548 (1998).
- “Disordered and ordered C<sub>28</sub> solids”, J. Kim, G. Galli, J. W. Wilkins, and A. Canning, J. of Chem. Phys. **108**, 2631 (1998).
- “Prediction of charge separation in GaAs/AlAs “Russian Doll” nanostructures,” J. Kim, L. W. Wang, and A. Zunger, Phys. Rev. B **56**, R15541 (1997).
- “Extended Si {311} defects,” J. Kim, J. Wilkins, F. Khan, and A. Canning, Phys. Rev. B, **55**, 16186 (1997).
- “Carbon superatom thin films,” A. Canning, G. Galli, and J. Kim, Phys. Rev. Lett. **78**, 4442 (1997).
- “Total energy global optimization using nonorthogonal localized orbitals,” J. Kim, F. Mauri, and G. Galli, Phys. Rev. B **52**, 1640 (1995).
- “Surface phonons of the Si(111)-7×7 reconstructed surface,” J. Kim, M.-L. Yeh, F. S. Khan, and J. W. Wilkins, Phys. Rev. B **52**, 14709 (1995).
- “Parallel decomposition of the tight-binding fictitious Lagrangian algorithm for molecular dynamics simulations of semiconductors,” M.-L. Yeh, J. Kim, and F. S. Khan, Comp. in Phys. **9**, 108 (1995).

## INVITED TALKS

- “Molecular dynamics simulation of large scale Si and C systems using tight-binding  $O(N)$  method”, Local orbital methods for large scale atomistic simulations, CECAM workshop, Lyon, France (July 1998).
- “Extended Si defects”, Electronic structure workshop at Pohang University of Science and Technology, Republic of Korea (May 1998); Physics of insulators, workshop at Aspen center for physics, Aspen, CO (June 1998).
- “Tight-binding quantum simulations for thousands of atoms”, APS March Meeting, Los Angeles, CA (Mar. 1998).
- “Parallel implementation of the Car-Parrinello fictitious Lagrangian algorithm,” The annual workshop on recent developments in electronic structure algorithms, ITP, Santa Barbara, CA (June 1994).

## CONTRIBUTED TALKS

- “Carbon-silicon complexes in bulk silicon: their roles in silicon diffusion,” MRS Meeting, Boston, MA (Nov. 1999).
- “Thermal properties of di-interstitial defects in silicon and their role in the growth of extended interstitial defects,” MRS Meeting, Boston, MA (Nov. 1999).

- “Dynamics simulations of extended defects,” APS March Meeting, Atlanta, GA (Mar. 1999).
- “Hyperdynamics of Si dimers diffusing on Si(001) surface.” APS March Meeting, Atlanta, (Mar. 1999).
- “Pseudopotential calculations of semiconductor nanostructures – Russian Doll GaAs/AlAs and strained InAs/GaAs,” APS March Meeting, Kansas City, MO (Mar. 1997).
- “Extended Si defects,” APS March Meeting, Kansas City, MO (Mar. 1997).
- “Simulations of C<sub>24</sub> collisions by orbital-based  $O(N)$  method,” The annual workshop on recent developments in electronic structure algorithms, St. Mary’s College of Maryland, MD (May 1995); APS March Meeting, St. Louis, MO (Mar. 1996).
- “Total energy global optimization using nonorthogonal localized orbitals,” APS March Meeting, San Jose, CA (Mar. 1995).
- “Surface phonons of the Si(111)-7×7 reconstructed surface,” APS March Meeting, Pittsburgh, PA (Mar. 1994).

## PERSONAL REFERENCES

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| Dr. Giulia Galli      | <i>Lawrence Livermore National Laboratory</i><br>P.O. Box 808, L-415<br>Livermore, CA 94551<br>e-mail: <a href="mailto:galli@modena.llnl.gov">galli@modena.llnl.gov</a>                                |
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