High Performance Algorithms for Electronic Materials

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Goals of Our Research Program

- ***The focus of our research is to exploit high performance computers for solving large scale and complex problems that arise in modeling real materials.***
- ***Our planned research efforts will center on electronic materials in the form of complex solids, atomic clusters, liquids, and glasses.***
- ***The means to accomplish this research will be based on a strong interdisciplinary program between computational and physical scientists.***

Program Overview

- Research Highlights
  - Algorithm Developments
  - Applications to Materials
    - Defects
    - Liquids
    - Clusters/quantum dots
  - Recent Publications
- Personnel, facilities, outreach

Algorithm Developments

- ***Real space*** description of pseudopotentials constructed with density functional theory (J.R. Chelikowsky, N. Troullier, and Y. Saad, Phys. Rev. Lett. 72, 1240 (1994))

  -Powerful approach: easy to implement on parallel platforms, ideally suited for localized systems.

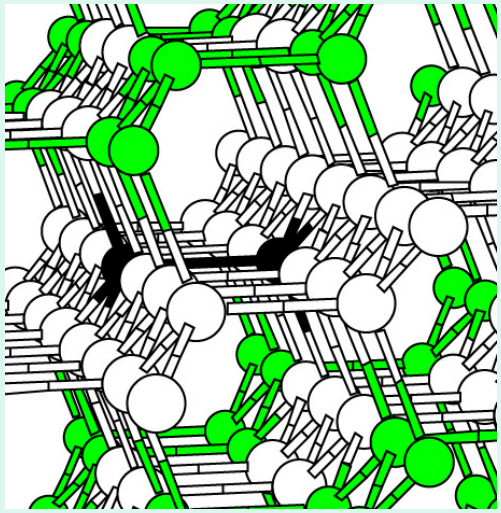
- ***Advances in algorithms***
  - Developed parallel finite difference code for real-space electronic structure problem
    - Structural energies, vibrational spectra
    - Ab initio molecular dynamics
    - Polarizabilites, dielectric response
    - Time dependent density functional theory
  - Parallel eigenvalue codes on various machines (Davidson)
  - Demonstrated the possibility of eigenvector-free methods in self consistent calculations.
  - Optimized the code for the IBM SP and other platforms

EXAMPLES OF APPLICATIONS

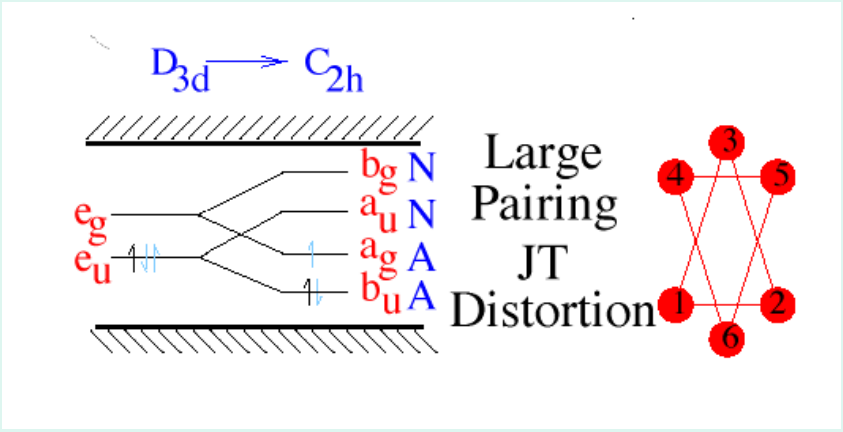
- Defects: Structure, energy levels
- Clusters: Polarizablity, photoemission, structure
- Quantum dots: Optical excitations, role of surface passivation, quantum confinement
- Liquids: Structure, electronic and optical properties, diffusion

Divacancy in Silicon

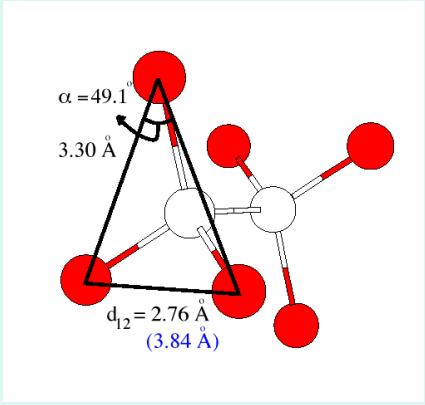
- Watkins using spin resonance methods proposed a model for explaining electronic energy levels in 1965 based on large Jahn-Teller (JT) distortion.
- Previous theoretical work was not consistent with his model. Our work is consistent.
- Only if large (more than a hundred atoms) systems are considered can one replicate his model.
- Real space methods and new computational platforms have allowed us to examine such size regimes.



Model of Divacancy

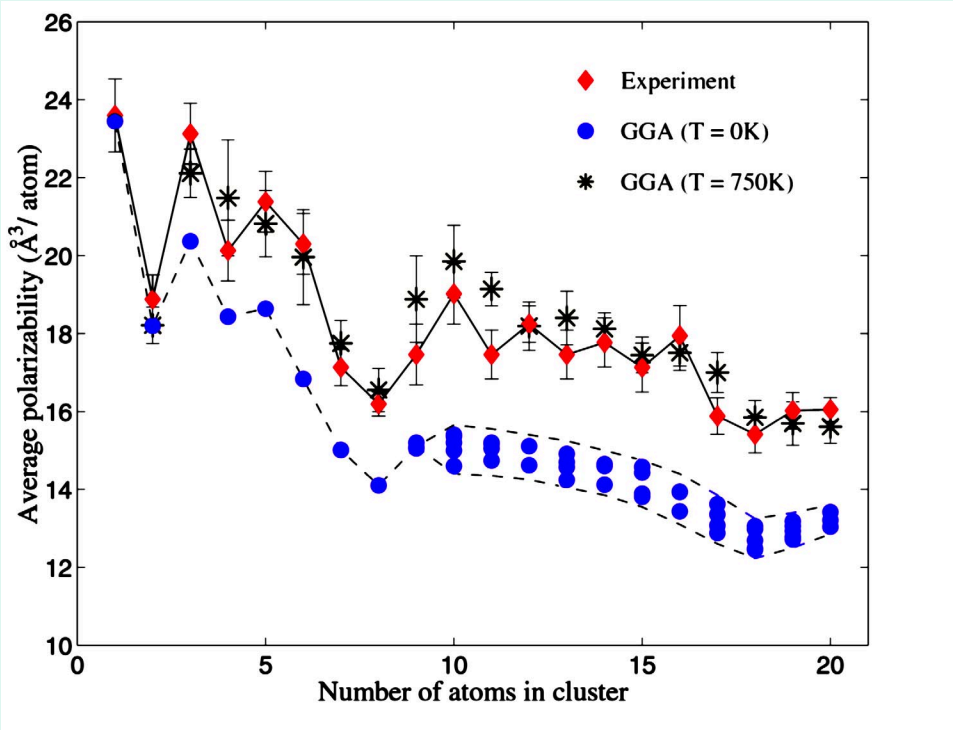


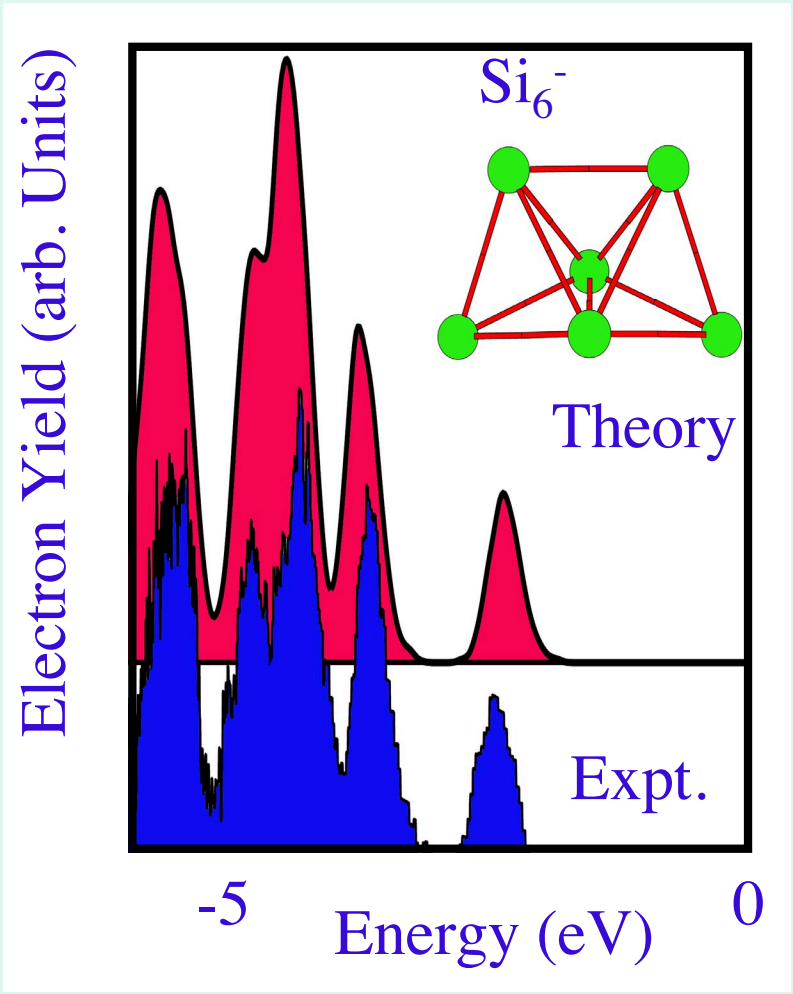
Energy structure levels and structure proposed by Watkins



Calculated structure showing large JT distortion

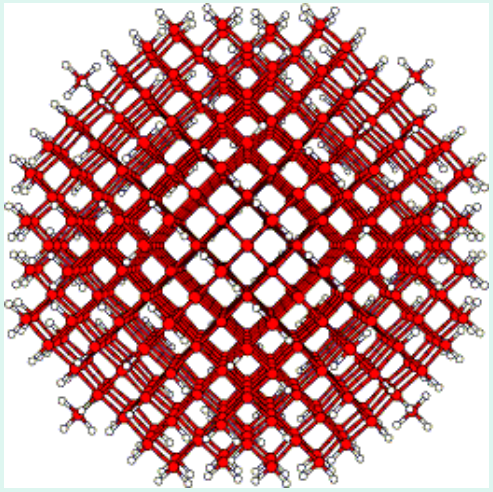
Photoemission and Polarizabilities of Localized Systems





Prior density functional theory calculations for the polarizability of Na clusters have been at variance with experiment. Using *finite* temperature ab initio molecular dynamics simulations, we resolved this discrepancy.

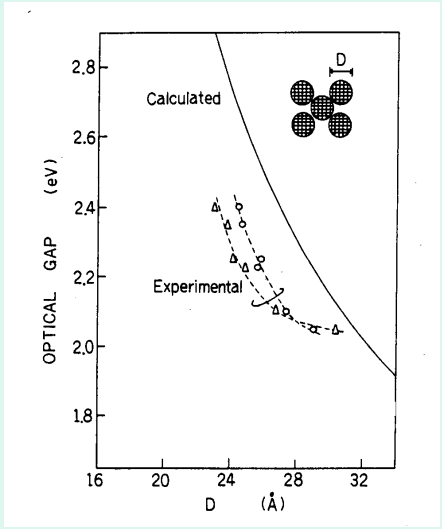
Compared calculated "density of states" from ab initio simulations have suggested that cluster anions are often not in the ground state. We proposed a new "rule" for predicting the observed spectra.



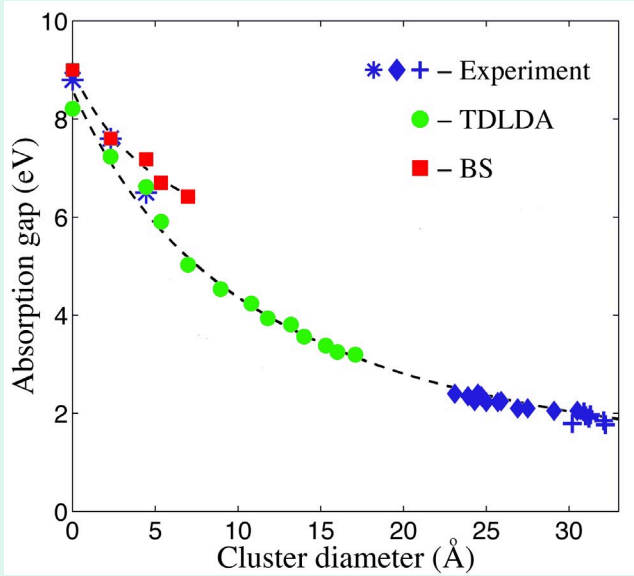
Optical Properties of Localized Systems

Implemented *time dependent density functional theory* to predict the role of quantum confinement in clusters (Si, GaAs, CdSe) and quantum dots.

Quantum dot



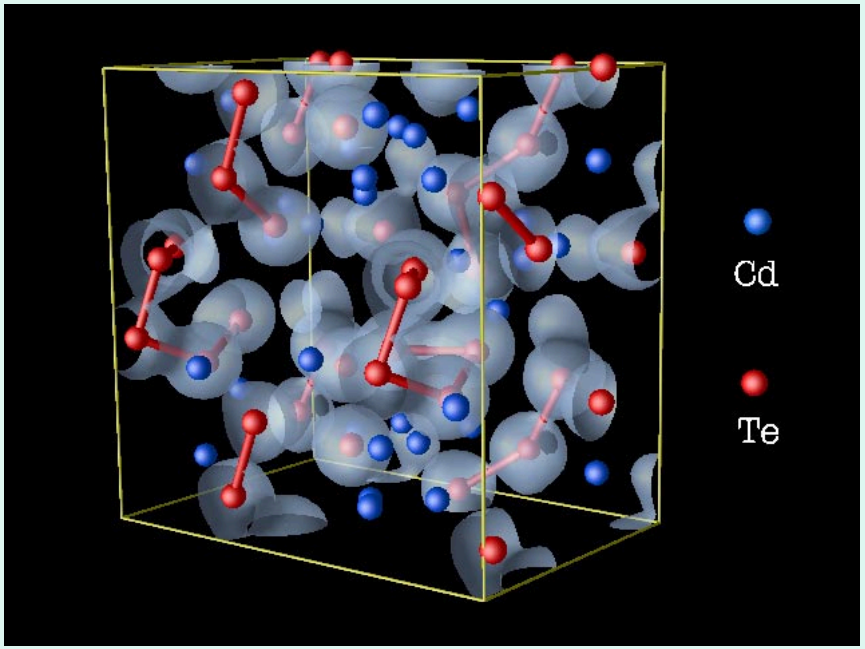
Example of quantum confinement



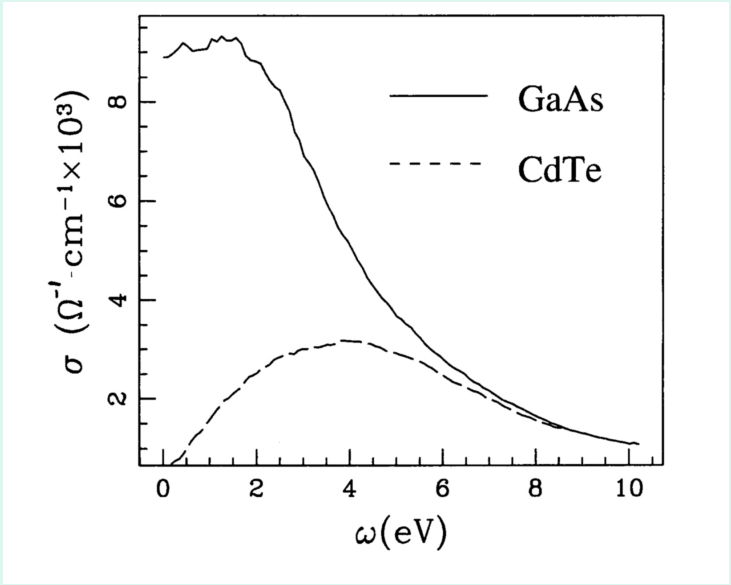
Comparison of calculated gaps from TDLDA to small hydrogenated molecules and quantum dots.

Electronic and Structural Properties of Semiconductor Liquids

•First studies of II-VI and IV-VI liquids.
- GeTe liquid shows anomalous "reentrant" Peierls Distortion
- CdTe prediction of optical conductivity as function of temperature



Ab initio simulation of liquid CdTe



Optical conductivity of liquid GaAs and CdTe. GaAs is a metal in the melt; CdTe is a semicondcutor

Recent Publications

- **Defects in solids: Divacancy in Silicon**
  - S. Ogut and J.R. Chelikowsky, Phys. Rev. Lett. **83**, 3852 (1999).

- **Liquid semiconductors: Optical and Structural Properties of Liquids**
  - V. Godlevsky, et al., Phys. Rev. Lett. **81**, 4959 (1998).
  - J.Y. Raty et al., Phys. Rev. Lett. **83**, 3852 (2000).

- **Optical and collective excitations in clusters, quantum dots and complex solids:**
  - I. Vasiliev, S. Ogut and J.R. Chelikowsky, Phys, Rev. Lett. **82**, 1919 (1999).
  - J. Muller, et al., Phys. Rev. Lett. **85**, 1666 (2000).
  - I. Vasiliev, S. Ogut and J.R. Chelikowsky, Phys, Rev. Lett. **86**, 1813 (2001).
  - L. Kronik, et al., J. Chem. Phys. **115**, 4322 (2001).
  - J. Woicik, et al., Phys. Rev. Lett. (2002), in press.

Future Research Directions

- **Algorithms**
  - Developing out-of core methods for the real-space method using polynomial filtering, eliminate eigenvalue problem.
  - Implement real space methods with periodic boundary conditions
  - Investigate techniques for reducing cost of time dependent density functional theory using different algorithms.

- **Physical Science**
  - Spintronics systems (magnetic semiconductors, GaMnAs, GaMnN, GaMnP): extended systems and quantum dots
  - Optical excitations in dots, clusters and molecular systems (Green Function, time dependent density functional theory)
  - Complex fluids and defects
  - Full dielectric matrix calculations for localized systems

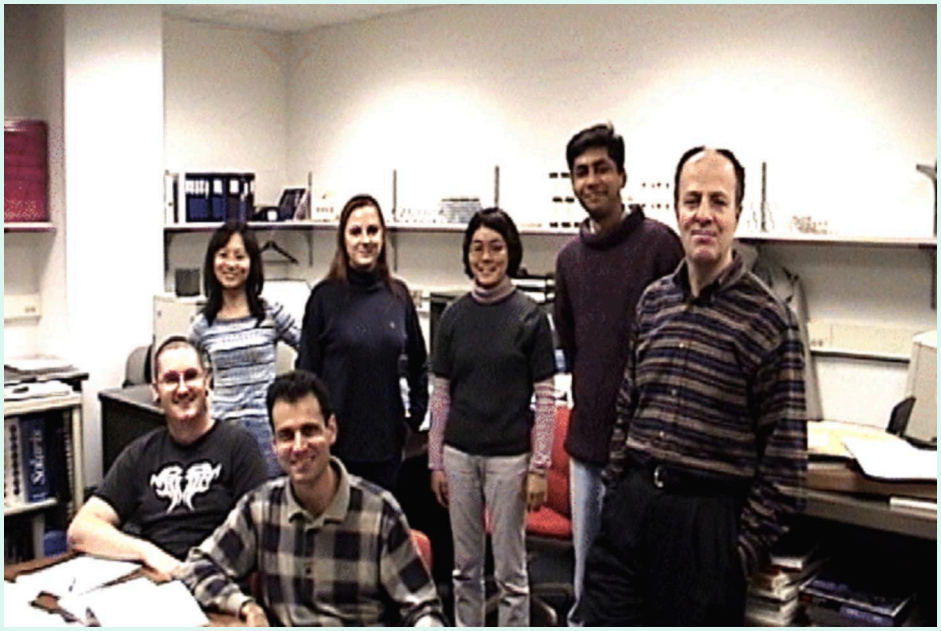
Personnel

Graduate Students

Physics: Eunjung Ko and Vitaliy Godlevsky (PhD, 99)
Materials Science: Igor Vasiliev (PhD, 00), Manish Jain (PhD, 02), Shen Li
Chemical Physics: Claudia Troparevsky
Scientific Computation: Russ Burdick (MS, 02)
Computer Science: Luis Yunes, Yu Liang, Laurent Smoch

Postdoctoral Fellows

Leeor Kronik, Manuel Maria Gonzalez Alemany, Emmanuel Lorin, Tajendra Vir Singh



Group at Minnesota

Left to right: First row- Russ Burdick and Leeor Kronik. Second row- Shen Li, Claudia Troparevsky, Eunjung Ko, Manish Jain and Yousef Saad.

Facilities and Programs at Minnesota

- Digital Technology Center
  - Supercomputing Institute for Digital Simulation and Advanced Computing
- MRSEC (Magnetic Heterostructures)
- IGERT (Nanoparticle Science and Engineering)

Web Sites

- **Software site**

  http://www-users.cs.umn.edu/~saad/software.html

  – Codes: SPMATH, SPARSKIT, Sparse matrix computations.

- **Research**

  http://jrc.cems.umn.edu/

  – Preprints, reprints and codes (PARSEC) real space pseudopotential; molecular dynamics and time dependent density functional theory.