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Integration of the Socorro Code into the NNIN/C Code Base

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Background

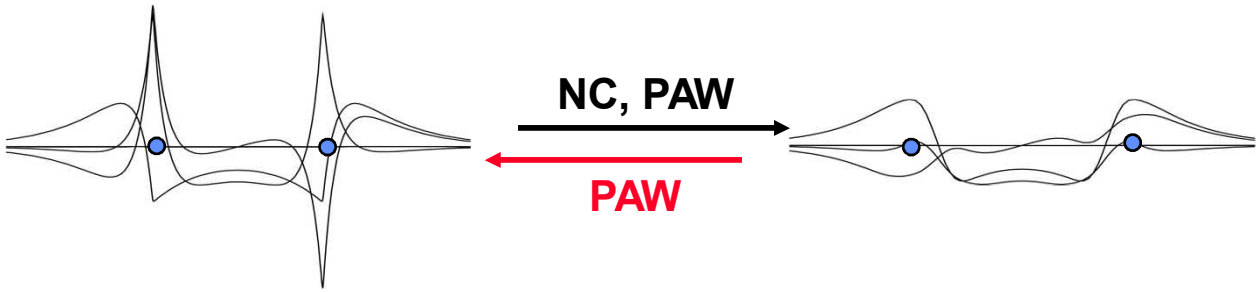
- *First-principles techniques based on density-functional theory (DFT) are important contributors to science, including nanoscience*
- *Developments in algorithms, math libraries, and parallel computers have enabled DFT studies of increasingly complex systems*
- *Increased reliance upon first-principles techniques provides impetus to improve DFT and techniques based on DFT*
- *More widespread use of DFT techniques has revealed inadequacies in DFT codes that impede the development of new techniques*
- ***Socorro** is our effort to provide a open-source electronic structure code which is highly efficient on parallel computers and easy to maintain*

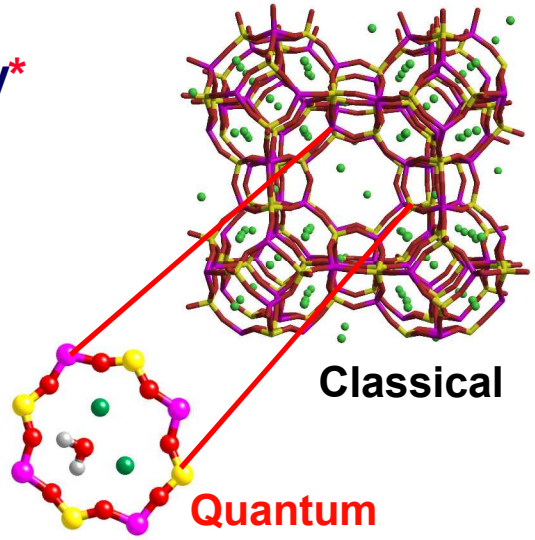
Socorro Software Design Features

- Open source (GNU public license)
  - researchers may use Socorro free of charge
  - developers may implement new techniques within Socorro
- Mainly written in Fortran 95 with a few parallelized C routines
- Powerful runtime support for parallel I/O, communication, and math operations
- Code consists of ≈ 40 modules (30 define objects, 10 provide support)
- Data is contained in derived (user-defined) types and organized hierarchically
- Support is provided for memory management (garbage collection)
- Unnecessary copying of large data structures is systematically avoided
- Computation and communication are separated for wavefunction FFT's

Socorro Capabilities

- Provides structures, energetics, transition states, and MD
- A full set of standard DFT code features with a plane wave basis set
- LDA, GGA (PW91, PBE, BLYP), AM05, and EXX* exchange-correlation
- Projector-Augmented Wavefunction (PAW) method
- Quantum Mechanics / Molecular Mechanics capability*
- Time-dependent DFT*





* Research level implementation

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Socorro and NNIN/C

- DOE ASC funded development of Socorro
  - Focused on specific national security problems

- Center for Integrated Nanotechnologies (CINT)
  - DOE National User Facility
  - User project to integrate Socorro into NNIN
  - Finite resources targeted in a specific area

- National Nanoscience Infrastructure Network
  - Provides access to greater community
  - Help with first line training and support

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Accomplishments

- Socorro running and tested on Harvard NNIN system
- Mike Stopa and Kaxiras group trained in running Socorro
- Mike Stopa modified Socorro to work with Condor
  - GOAL: Provide Socorro as a grid service

- Maria Fyta visited CINT and learned to run EXX calculations
- Looking forward to porting to more NNIN machines

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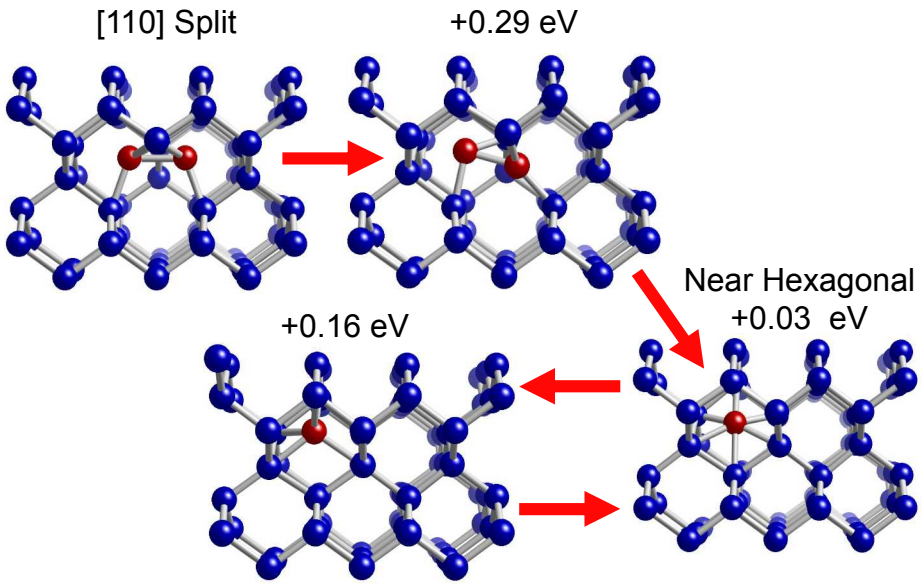
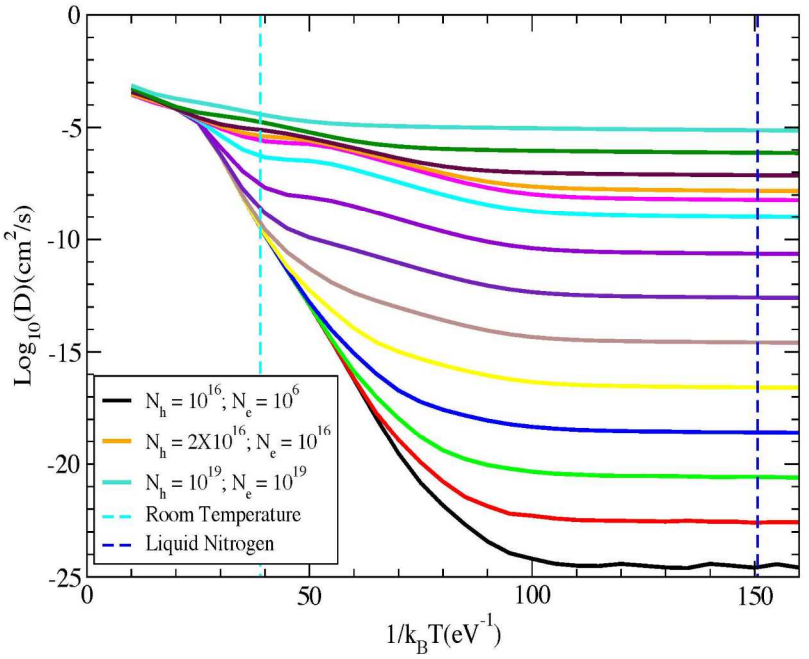
An Example: Atomistic Behavior of Semiconductor Defects

Experiments yield almost no information about the Silicon Self-Interstitial!

Socorro calculations were used to determine structures, pathways, and reaction barriers for the Si Self-Interstitial

Kinetic Monte-Carlo calculations based on the DFT results were used to determine the diffusion coefficient





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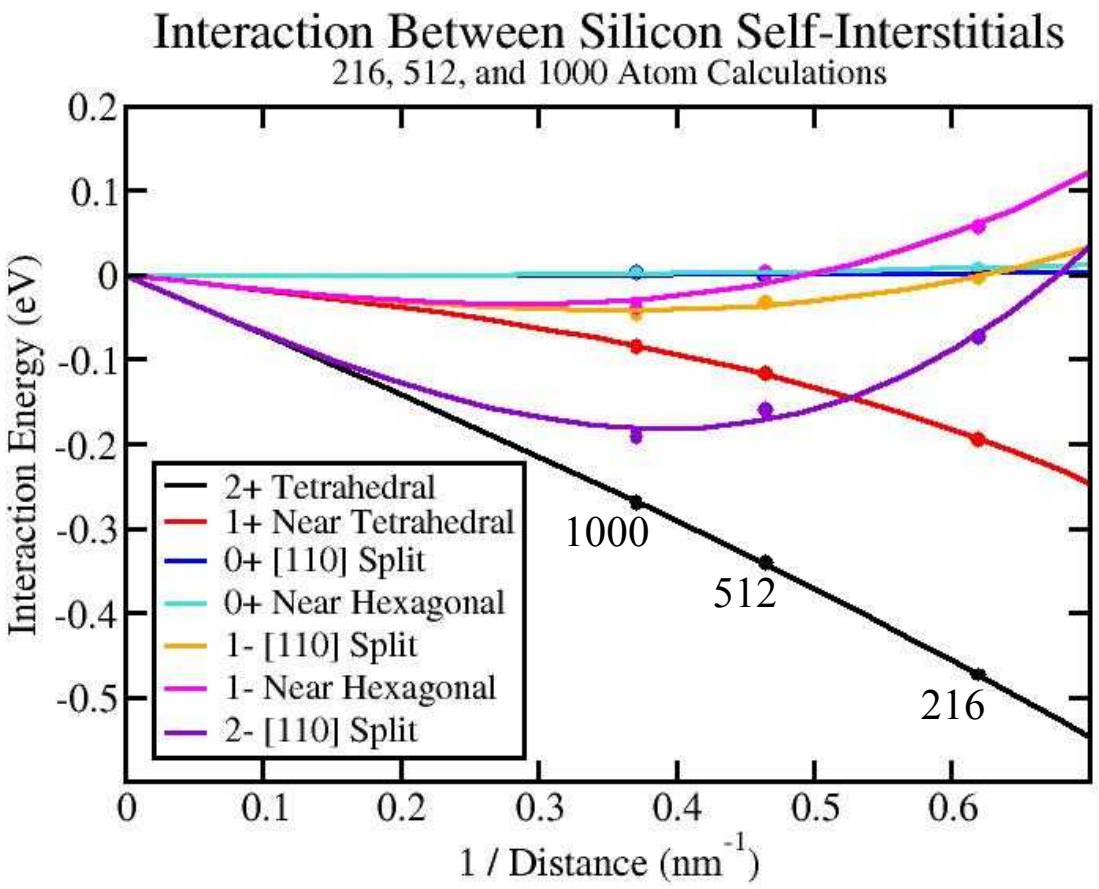
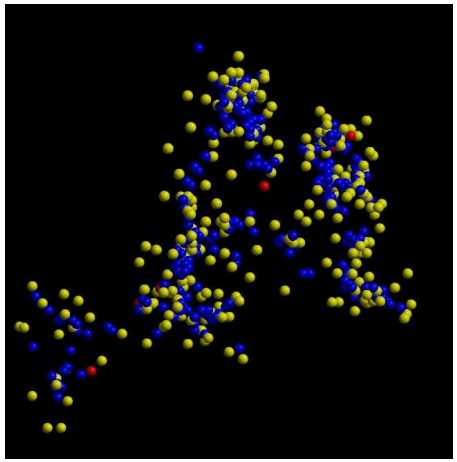
Socorro Used to Explore Defect Interactions at the Nanoscale



- **Perform DFT calculations for a cubic lattice of defects (Si self-interstitials)**
- **Vary the distance between defects by varying the supercell size**



Defect cluster from MD by Steven Foiles

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An Exciting New Socorro Capability: The Exact Exchange Approximation (EXX)

- Consider an energy functional $E(\phi_1,\ldots,\phi_N)$
- Constrain $\phi_1,\ldots,\phi_N$ to be solutions of the Kohn-Sham Eq.

$$H\phi_i = (K + V_I + V)\phi_i = \varepsilon_i\phi_i$$

- Minimize E with respect to the local potential V
- EXX takes E to be the Hartree-Fock energy

$$E_{EXX} = \sum_i \left\langle \phi_i^* (K + V_I)\phi_i \right\rangle + e^2 \iint \frac{\sum_{i,j} \left\{ \phi_i^*(r)\phi_i(r)\phi_j^*(r')\phi_j(r') - \phi_i^*(r)\phi_i(r')\phi_j^*(r')\phi_j(r) \right\}}{|r - r'|} dr dr'$$

- V, ϕ_I are functionals of the density ρ, so EXX is DFT

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A New Algorithm for EXX Calculations Using A Plane Wave Basis

- Developed and implemented a new algorithm for EXX calculations based on a gradient based iterative minimization of the energy.

- Based on earlier work of Hyman, Stiles, and Zangwill, Phys. Rev. B 62, 15521 (2000) and Kümmel and Perdew, Phys. Rev. Lett. 90, 43004 (2003).

- Enables EXX calculations for systems with up to a few hundred atoms at zero or finite temperatures

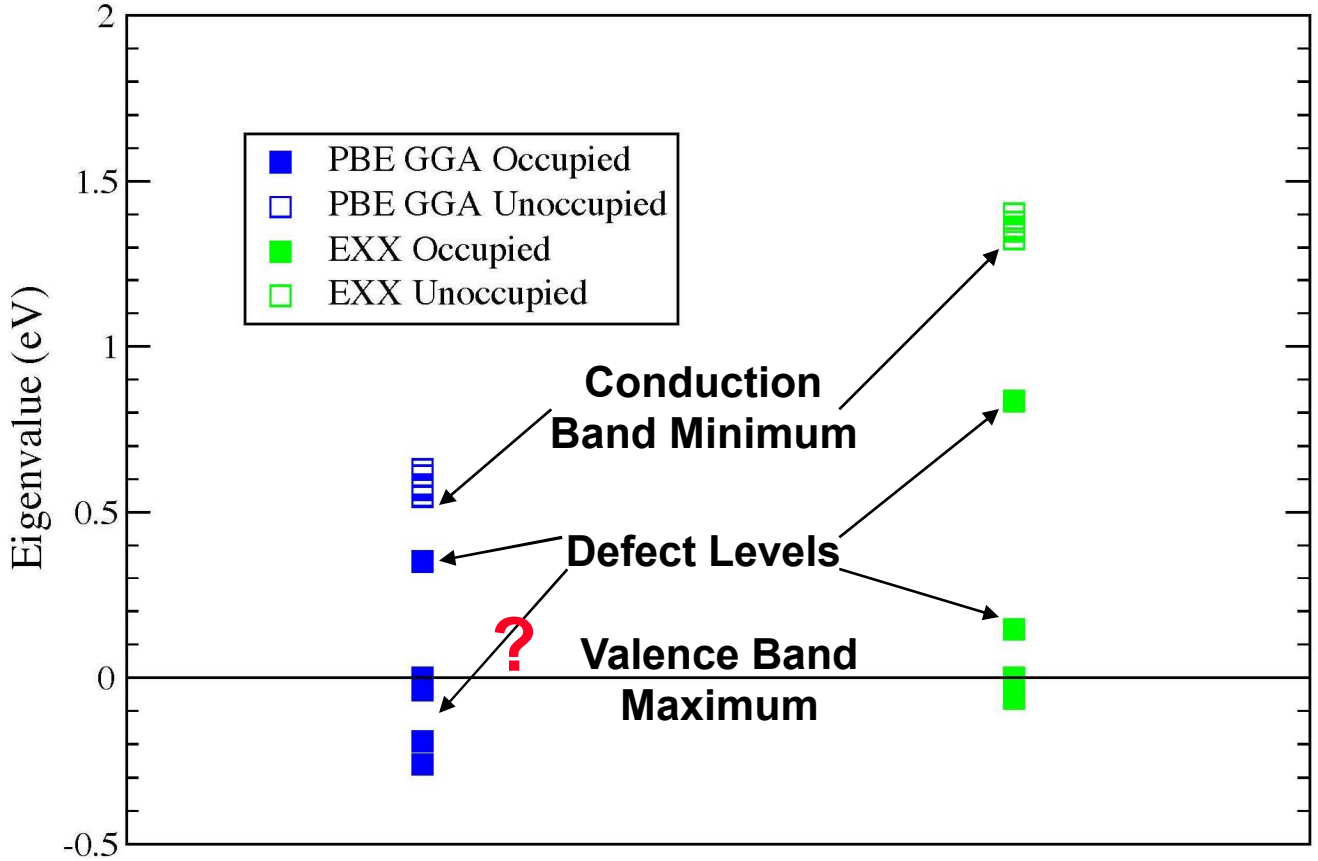
Our results agree with previous EXX calculations using more expensive methods

Property	Our EXX	Other EXX*	Experiment
Si Band Gap	1.28 eV	1.23 eV *	1.17 eV
Ge Band Gap	0.72 eV	0.94 eV *	0.66 eV
C Band Gap	5.09 eV	5.06 eV **	5.47 eV

* M. Städele et al, Phys. Rev. B 59, 10031 (1999).
** M. Städele et al, Phys. Rev. Lett. 79, 2089 (1997).

KLI pseudopotentials from FHI code for Si and Ge.

An Example EXX Application: Semiconductor Defect Calculations



- Si Self-Interstitial defect in 217 atom supercell
- -2 Charge state of Si_I should have two filled levels in the band gap
- Misplaced levels due to band gap problem sometimes lead to errors in total energies of charged states

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