Quantum mechanical predictions of defect properties for realistic device simulations

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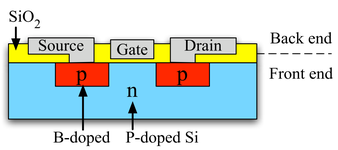
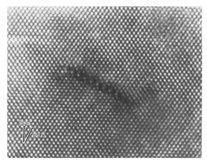
Introduction: Defects in Silicon Devices

- Ion implantation-induced interstitials precipitate extended defects
- Extended defects facilitate the broadening of doping profiles, which limits device size
- Radiation damage in space technology
- Experiments indicate the need for accurate defect simulations [2]





"Extended {311} Defect [1]"

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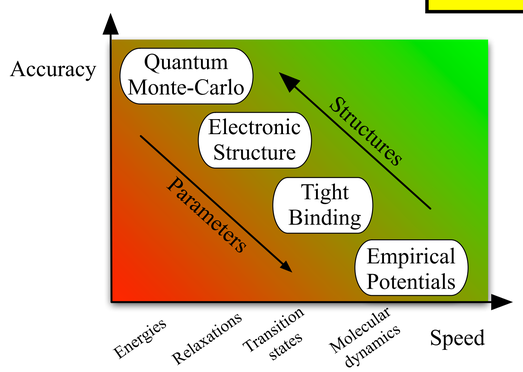
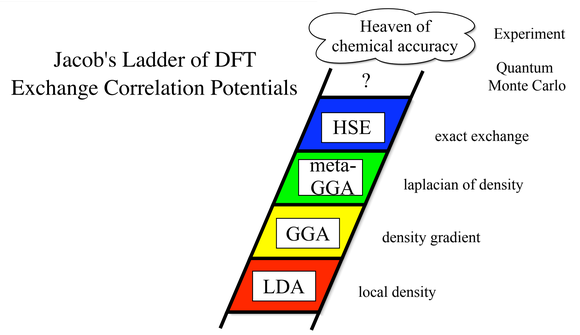
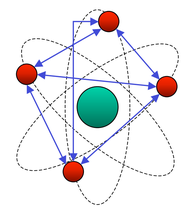
Methods: A Multiscale Approach







Transition state methods identify defect geometries → Electronic structure methods refine geometries and pathways → QMC determines accuracy of atomistic parameters

Molecular dynamics and dimer method
- Provides candidate structures for defects and saddle points [6]

Nudged Elastic Band Method
- Identifies defects and energy barriers

Transition State Theory
- Calculates transition rates

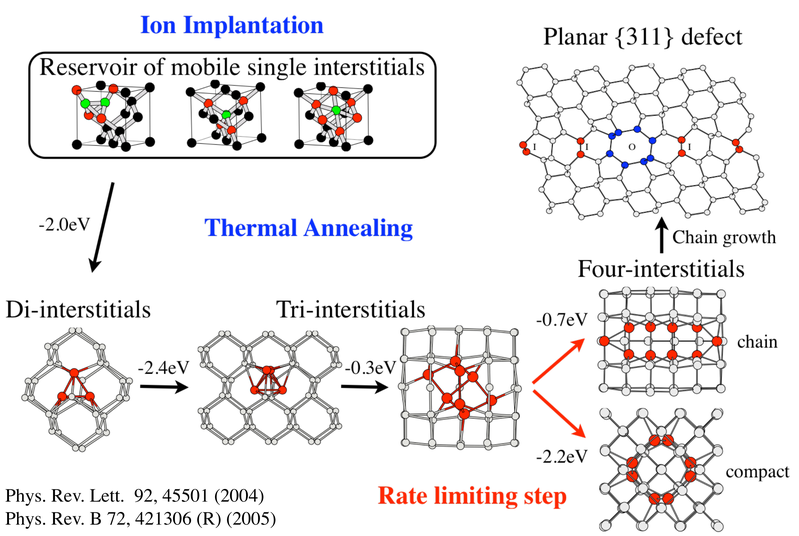
Hohenberg-Kohn Theorem (1964)

The ground state energy given by its electron density $n(r)$.
- Nobel prize in chemistry 1998 (Kohn and Pople)
- Most widely used "first principles" method

Checking the accuracy of the unknown density functional
- Climbing "Jacob's ladder" to heaven of chemical accuracy [3]
- Comparison to experiment or quantum chemistry
- Benchmark calculations by quantum Monte Carlo

- Stochastic solution of the many-body Schrodinger equation
- Explicitly includes electron-electron correlation and exchange via many-body wavefunctions
- **Variational Monte Carlo:** Optimizes the wavefunction by energy minimization [4].
- **Diffusion Monte Carlo:** Solves imaginary time Schrodinger equation and projects out the ground state [5].

Defect Evolution: From Point to Extended



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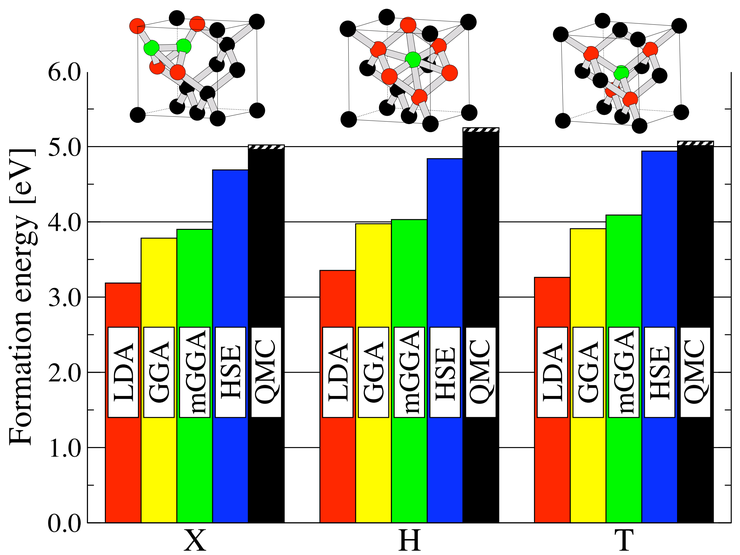
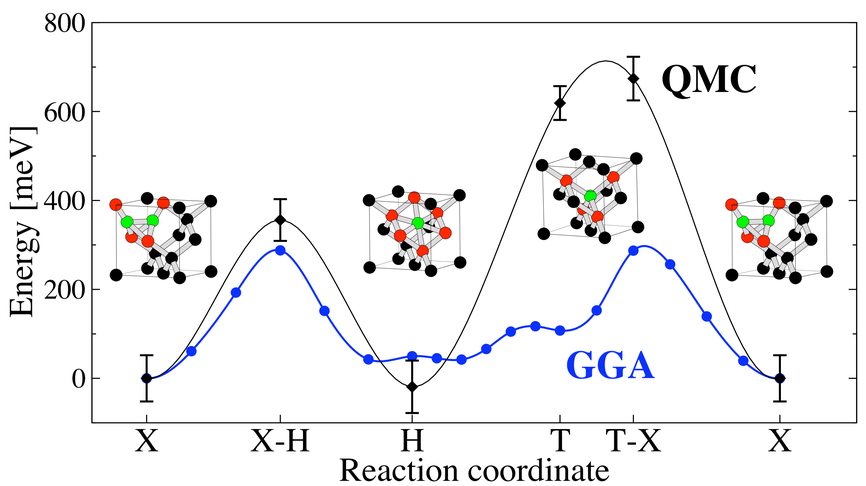
Mobile single interstitials first precipitate small compact defects and then larger, extended clusters. The compact four-interstitial can frustrate the growth of extended structures.

Single Interstitial Formation Energies:



Climbing "Jacob's ladder" of density functionals improves the accuracy for defect formation energies. The highest rung–hybrids–agree with QMC.

Interstitial Diffusion Barriers



Lowest energy barrier from X to H defect is similar in QMC and DFT. The T defect and its barrier are higher in QMC.