# OpenAtom: Fast, fine grained parallel electronic structure software for materials science, chemistry and physics.


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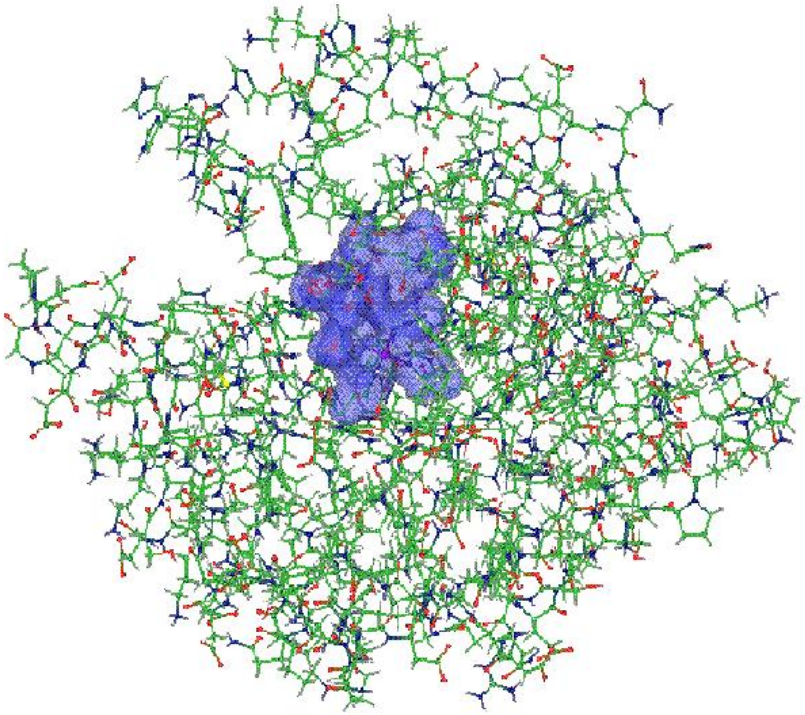
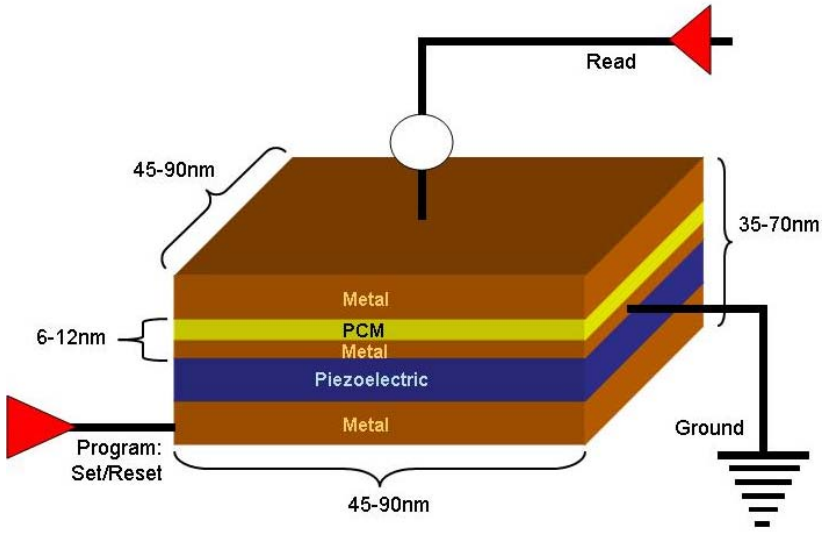
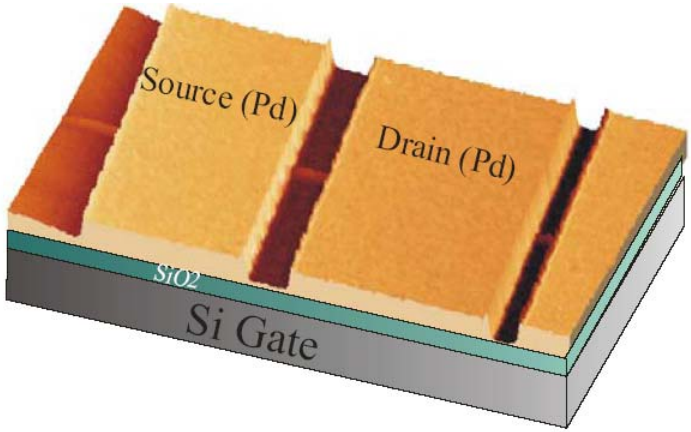
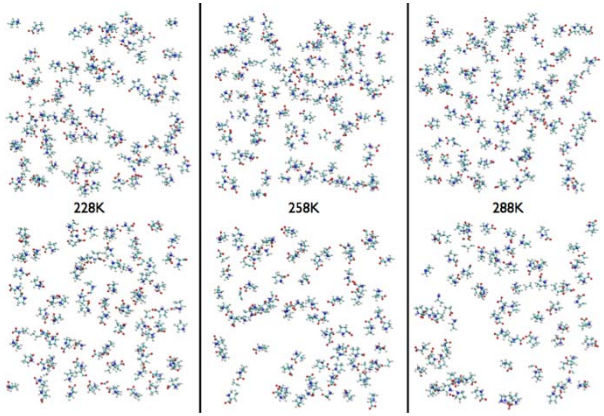
Funding : NSF, IBM Research, ONRL, …

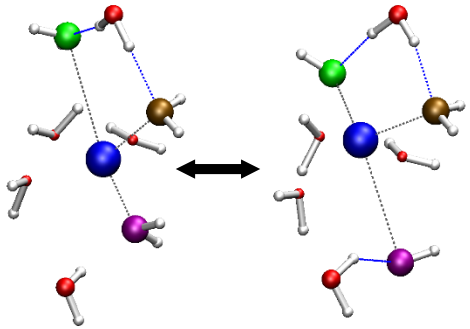
# Goal : The accurate treatment of complex heterogeneous systems to gain physical insight.





# Limitations of *ab initio* MD

- Limited to small systems (100-1000 atoms)*.
- Limited to short time dynamics and/or sampling times.
- Parallel scaling only achieved for

**# processors <= # electronic states**

until recent efforts by ourselves and others.

**Improving this will allow us to sample longer and learn new physics.**

*The methodology employed herein scales as $O(N^3)$ with system size due to the orthogonality constraint, only.

# Density Functional Theory : DFT

In the Kohn-Sham formulation of density functional theory, the electron density is expanded in a set of orbitals, $\{\psi_i(\mathbf{r})\}$,

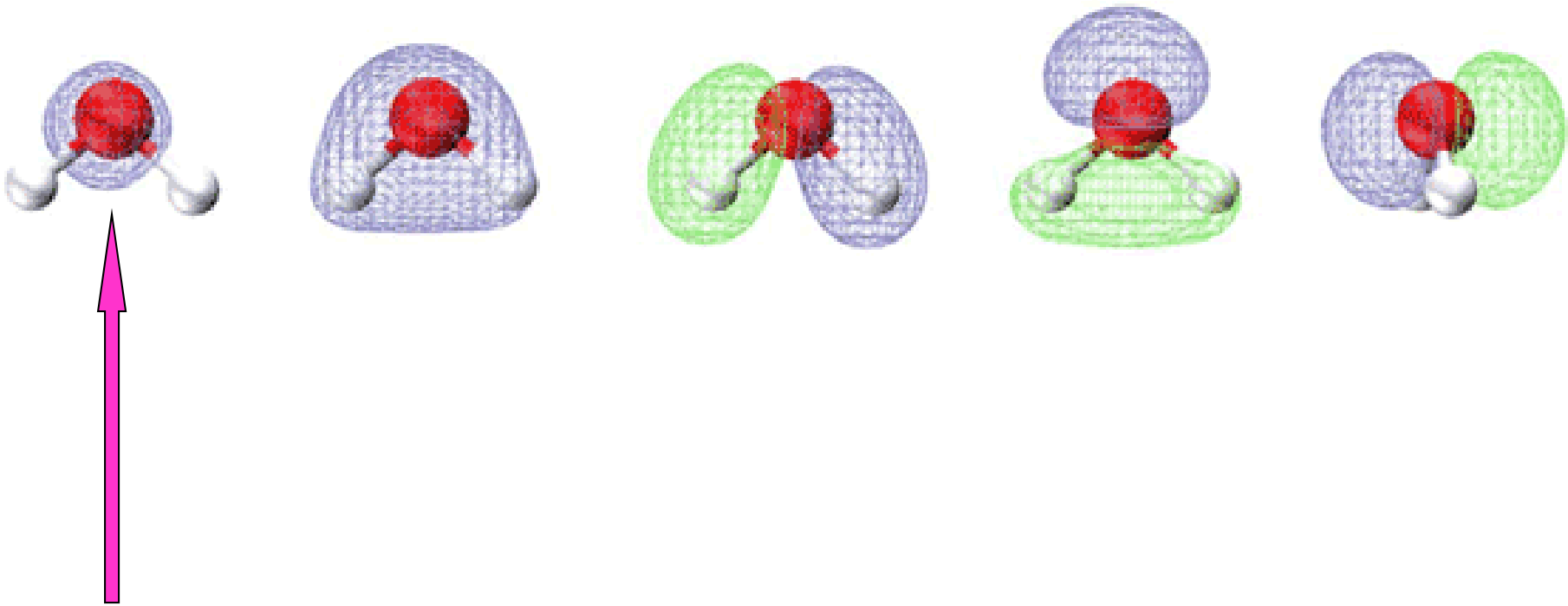
$$n(\mathbf{r}) \;=\; \sum_{i=1}^{n_{\rm occ}} f_i |\psi_i(\mathbf{r})|^2$$

subject to the orthogonality constraint, $(\langle\psi_j|\psi_k\rangle = \delta_{jk})$, where $n_{\rm occ}$ is the number of occupied orbitals and the $f_i$ are the occupation numbers.

The energy functional is given by

$$E[n] \;=\; T_s[\{\psi_i\}] + E_{\rm H}[n] + E_{\rm ext,loc}[n] + E_{\rm ext,non-loc}[\{\psi_i\}] + E_{\rm xc}[n]$$

# Electronic states/orbitals of water



Removed by introducing a non-local electron-ion interaction.

# Plane Wave Basis Set:

In plane-wave based calculations at the Γ-point, the orbitals and, hence, the density are expanded

$$\psi_i(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{g}} \bar{\psi}_i(\mathbf{g}) \exp(i\mathbf{g}\cdot\mathbf{r})$$

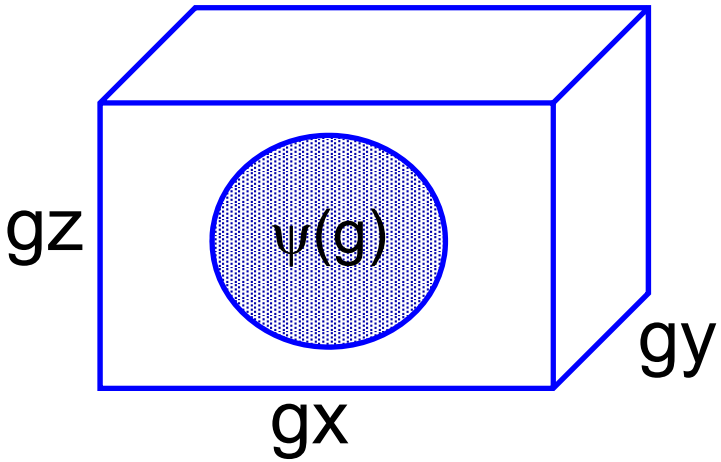
$$n(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{g}} \bar{n}(\mathbf{g}) \exp(i\mathbf{g}\cdot\mathbf{r})$$

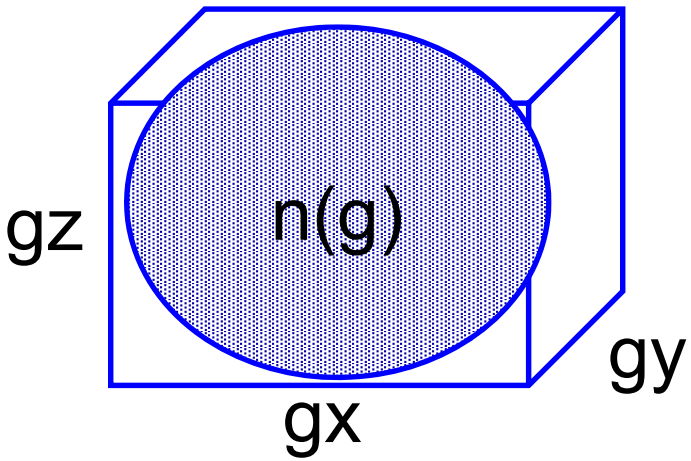
Here, $\hat{\mathbf{g}}$ is the vector of integers $\{j,k,m\}$, $\mathbf{g} = 2\pi\hat{\mathbf{g}}\mathbf{h}^{-1}$, $V = \det \mathbf{h}$ is the volume, $\mathbf{h}$ is the matrix whose columns are the Cartesian components of the three vectors describing the parallelepiped enscribing the system and $\mathbf{r} = \mathbf{hs}$. A plane wave basis can be used to described

The # of states or orbitals ~ N where N is # of atoms.
The # of pts in g-space ~N.
The # of electrons ~ N.

# Plane Wave Basis Set:

## Two Spherical cutoffs in G-space



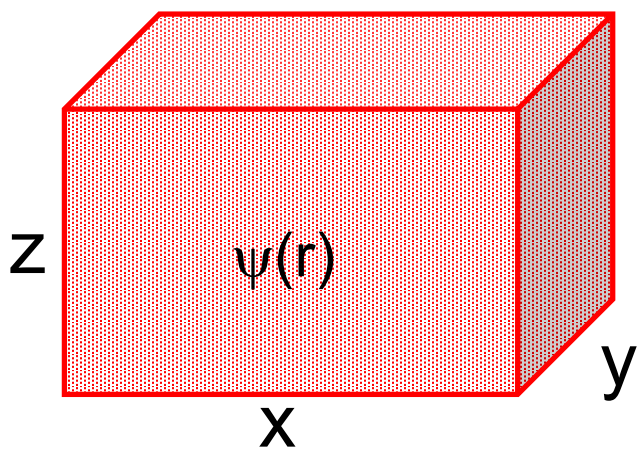

$\psi(g)$ : radius $g_{cut}$

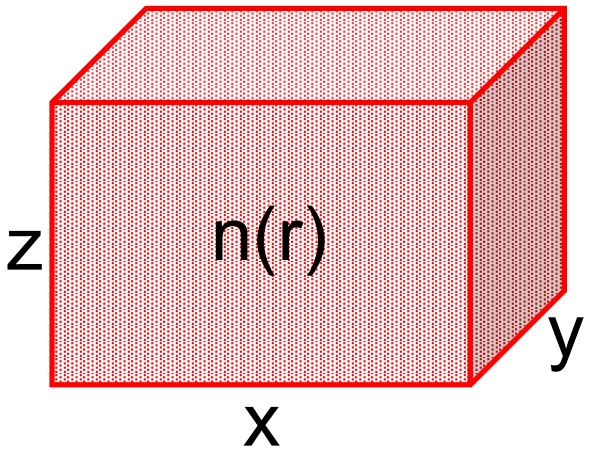
$n(g)$ : radius $2g_{cut}$

*g-space is a discrete regular grid due to finite size of system!!*

# Plane Wave Basis Set:

## The dense discrete real space mesh.



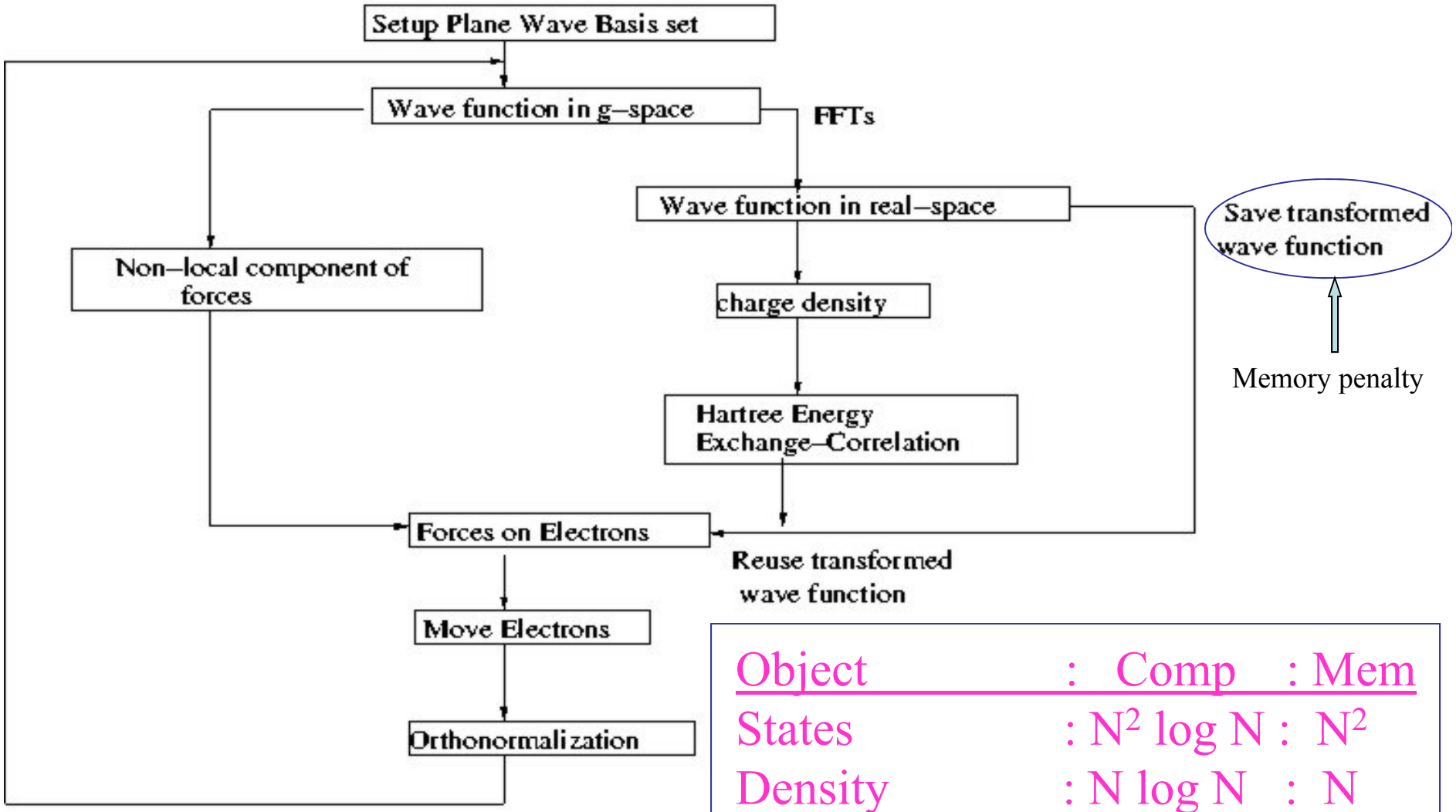

$\psi(r) = \text{3D-FFT}\{ \psi(g)\}$

$n(r) = \Sigma_k |\psi_k(r)|^2$

$n(g) = \text{3D-IFFT}\{n(r)\}$ exactly!

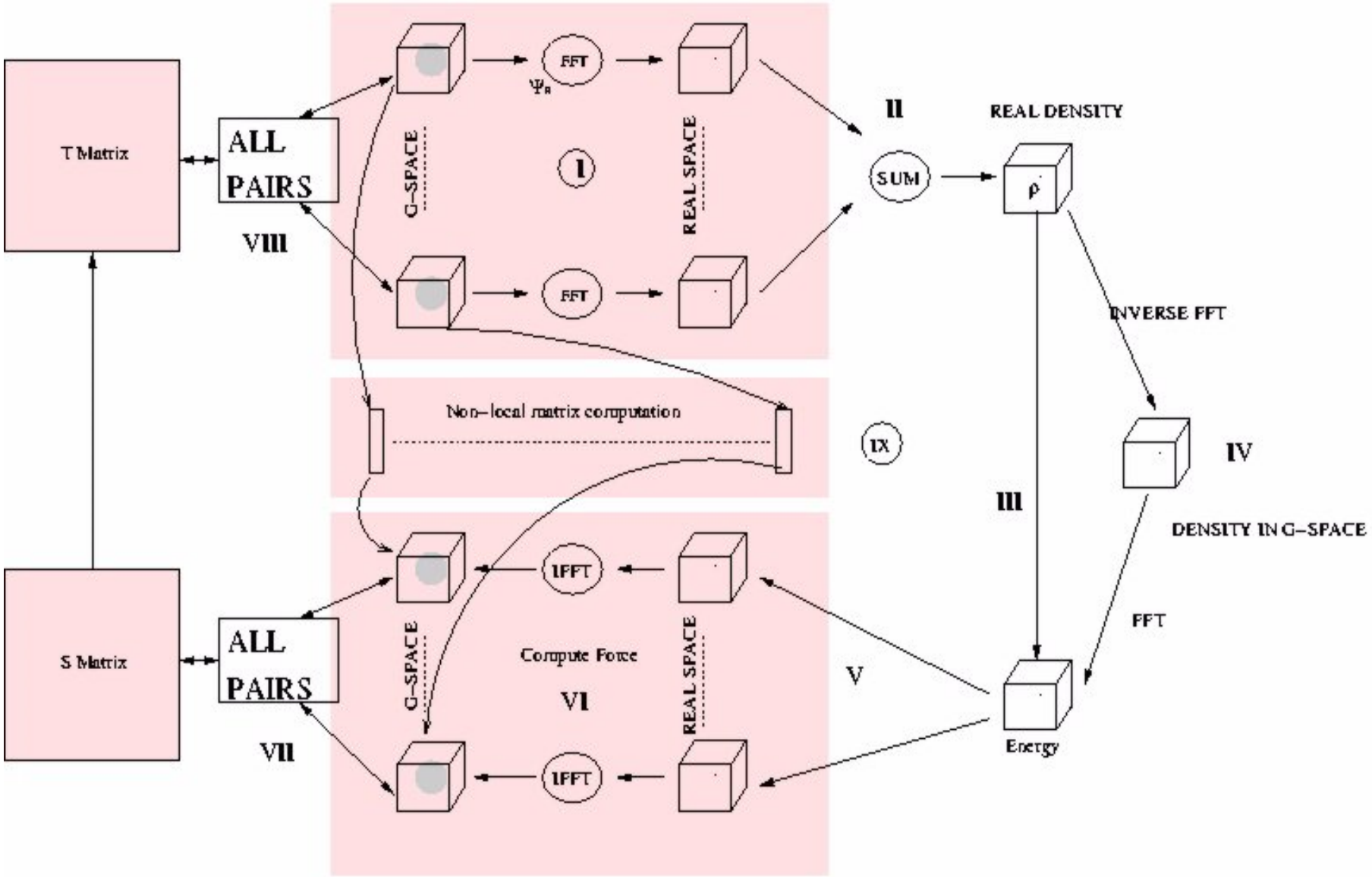
Although r-space is a discrete dense mesh, n(g) is generated exactly!

# Simple Flow Chart : Scalar Ops

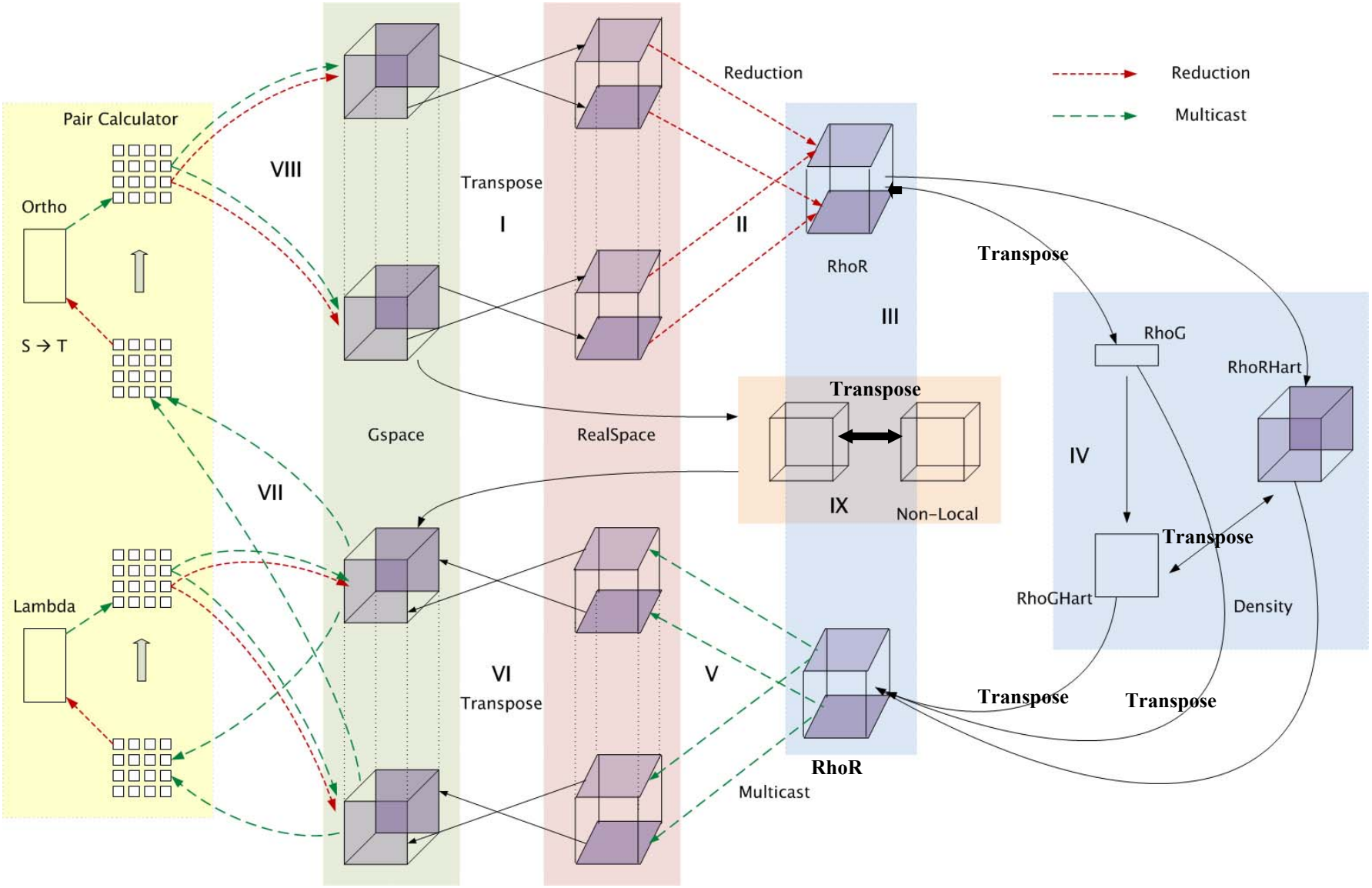



| Object | : Comp | : Mem |
|---|---|---|
| States | : $N^2 \log N$ | : $N^2$ |
| Density | : $N \log N$ | : $N$ |
| Orthonormality | : $N^3$ | : $N^{2.33}$ |

# Flow Chart : Data Structures



# Parallelization under charm++

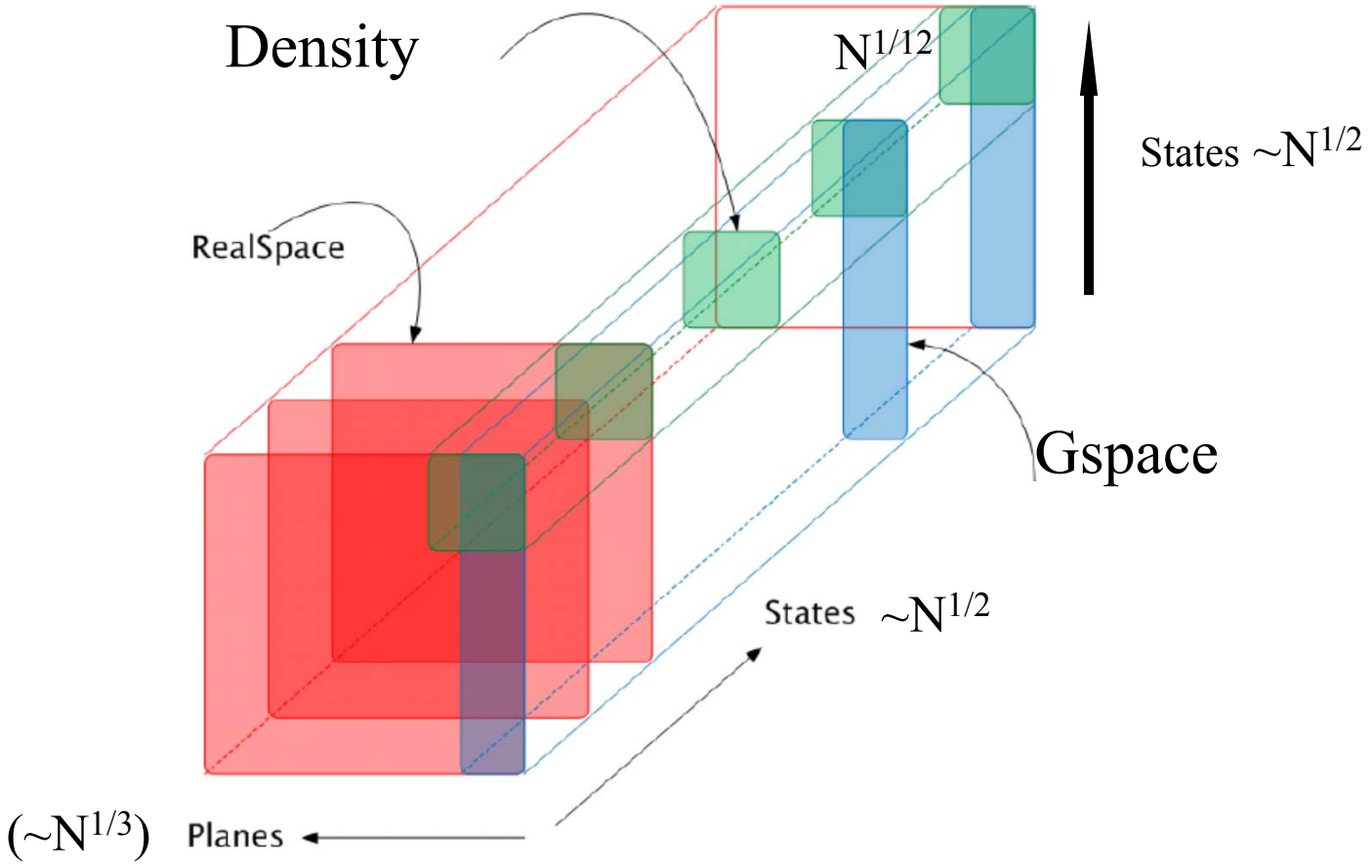


# Challenges to scaling:

- Multiple concurrent 3D-FFTs to generate the states in real space require AllToAll communication patterns. Communicate $N^2$ data pts.
- Reduction of states (~$N^2$ data pts) to the density (~N data pts) in real space.
- Multicast of the KS potential computed from the density (~N pts) back to the states in real space (~N copies to make $N^2$ data).
- Applying the orthogonality constraint requires $N^3$ operations.
- Mapping the chare arrays/VPs to BG/L processors in a topologically aware fashion.

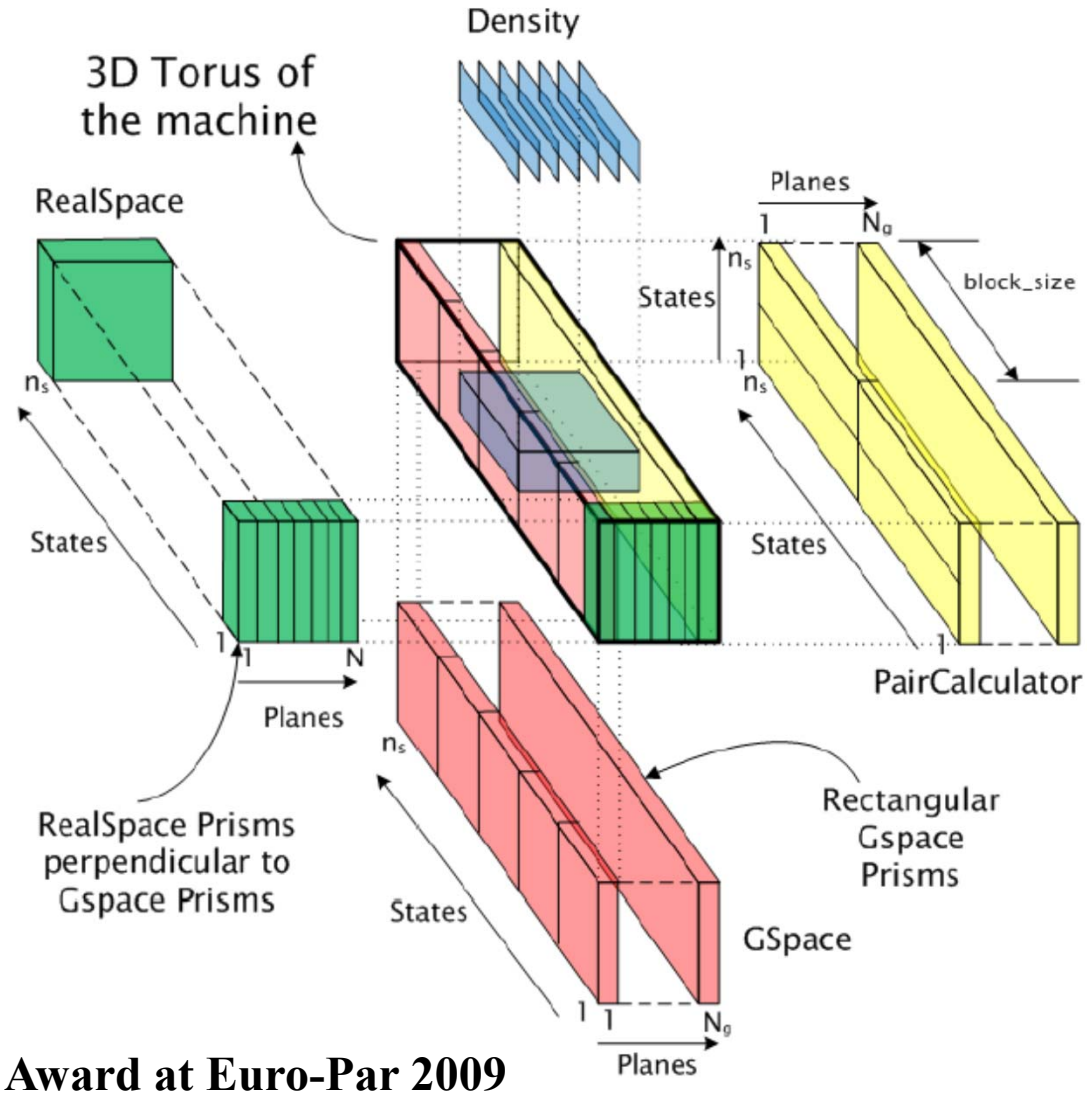
Scaling bottlenecks due to non-local and local electron-ion interactions removed by the introduction of new methods!

# Topologically aware mapping for CPAIMD



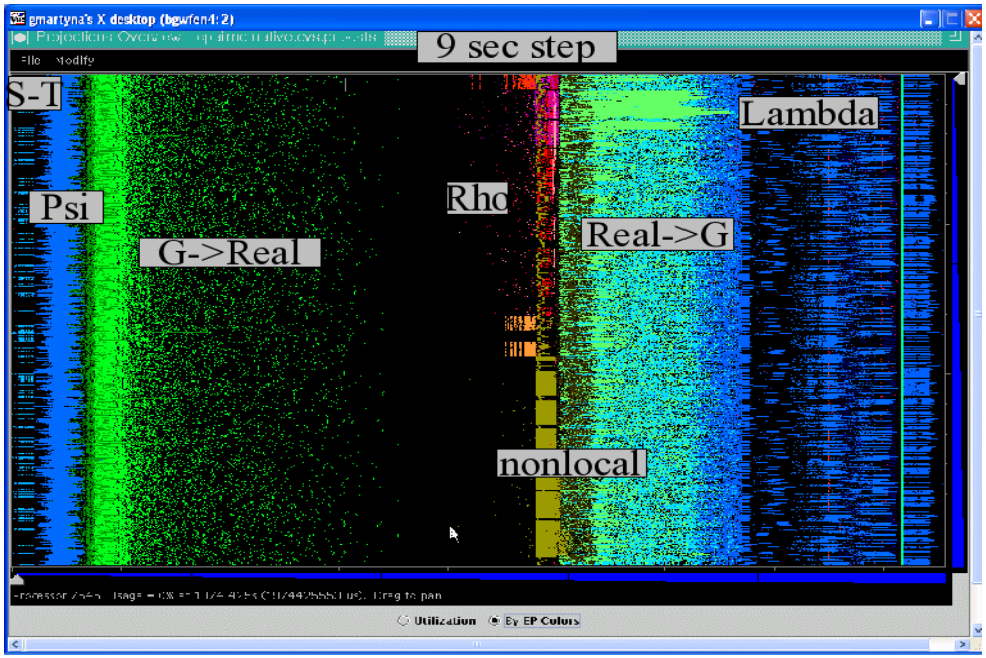

- The states are confined to rectangular prisms cut from the torus to minimize 3D-FFT communication.
- The density placement is optimized to reduced its 3D-FFT communication and the multicast/reduction operations.

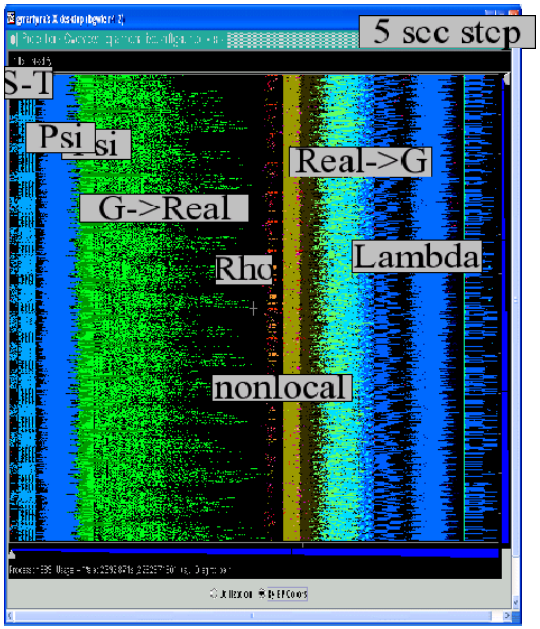
# Topologically aware mapping for CPAIMD : Details

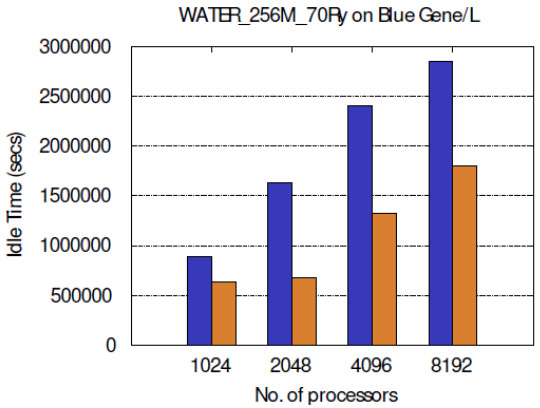


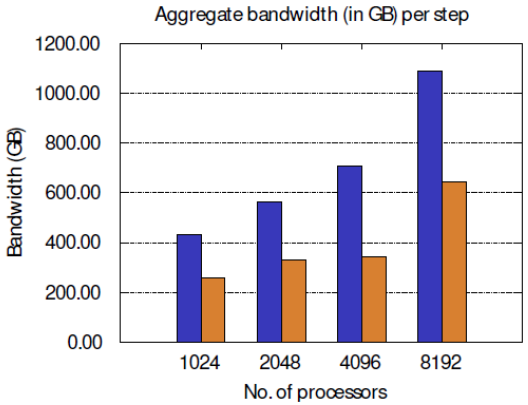

**Distinguished Paper Award at Euro-Par 2009**

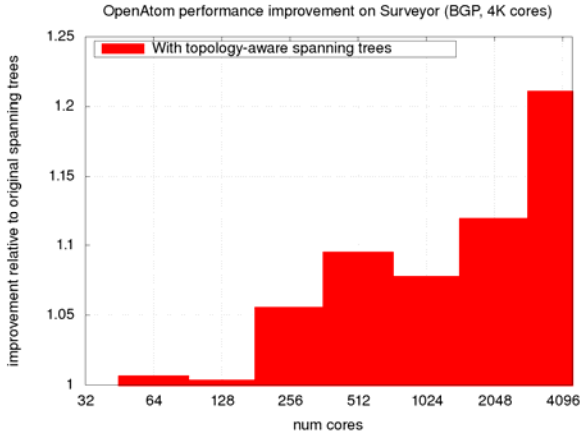
# Improvements wrought by topological aware mapping on the network torus architecture




Density (R) reduction and multicast to State (R) improved.
State (G) communication to/from orthogonality chares improved.

# Parallel scaling of liquid water* as a function of system size on the Blue Gene/L installation at YKT:

| CO Mode Native Layer with Optimizations | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Nodes | 32 | 64 | 128 | 256 | 512 | 1024 | 2048 | 4096 | 8192 | 16384 | 20480 |
| Processors | 32 | 64 | 128 | 256 | 512 | 1024 | 2048 | 4096 | 8192 | 16384 | 20480 |
| W8 Time s/step | 0.22 | 0.10 | 0.082 | 0.071 | 0.046 | 0.026 | 0.020 | | | | |
| W16 Time s/step | 0.73 | 0.40 | 0.23 | 0.15 | 0.106 | 0.061 | 0.041 | 0.035 | | | |
| W32 Time s/step | 2.71 | 1.52 | 0.95 | 0.44 | 0.26 | 0.15 | 0.11 | 0.081 | 0.063 | | |
| W64 Time s/step | | 6.72 | 3.77 | 1.88 | 0.87 | 0.51 | 0.31 | 0.21 | 0.15 | | |
| 128 Time s/step | | | | | 6.9 | 2.73 | 1.40 | 0.91 | 0.58 | 0.37 | 0.3 |
| W256 Time s/step | | | | | | 16.4 | 8.14 | 4.83 | 2.75 | 1.71 | 1.54 |

*Liquid water has 4 states per molecule.

- Weak scaling is observed!
- Strong scaling on processor numbers up to ~60x the number of states!
- IBM J. Res. Dev. (2009).

# Software : Summary

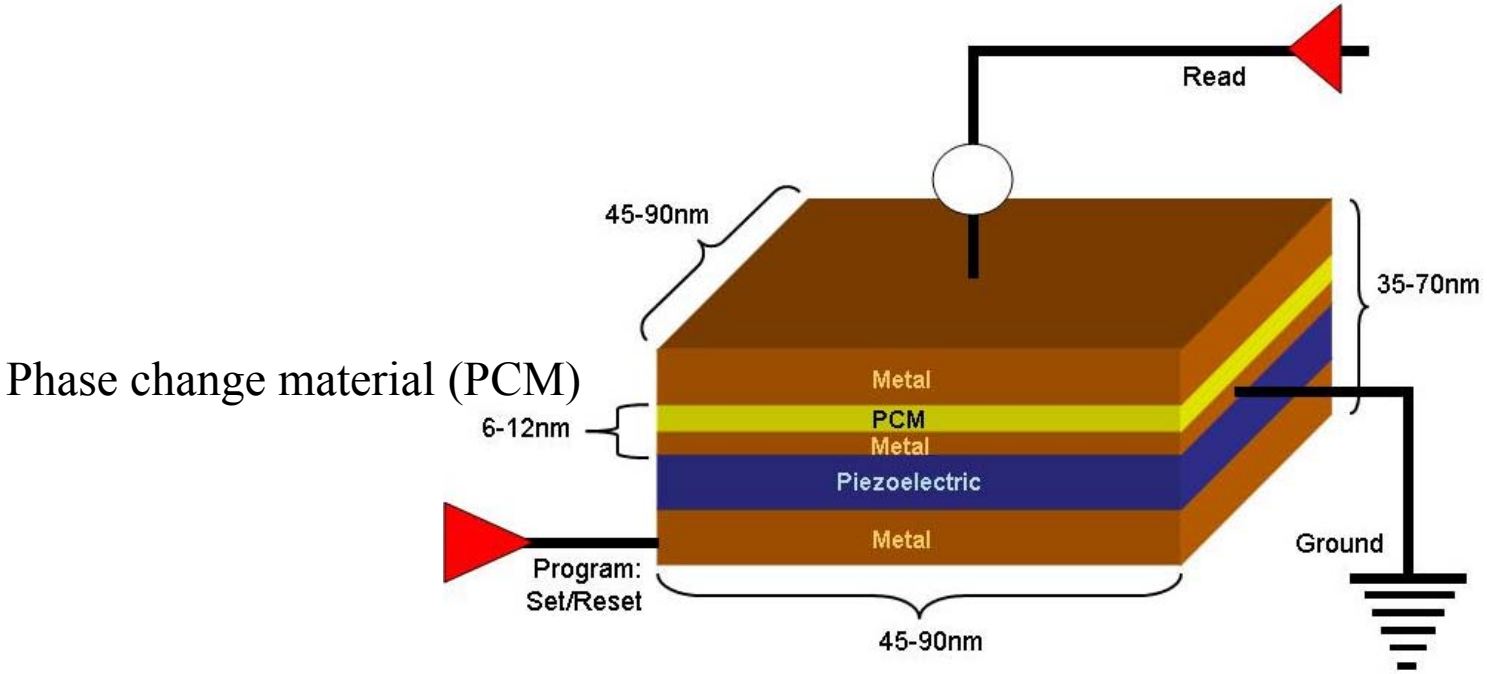
- Fine grained parallelization of the Car-Parrinello *ab initio* MD method demonstrated on thousands of processors :

  **# processors >> # electronic states**.

- Long time simulations of small systems are now possible on large massively parallel supercomputers.

# Application Study if time allows

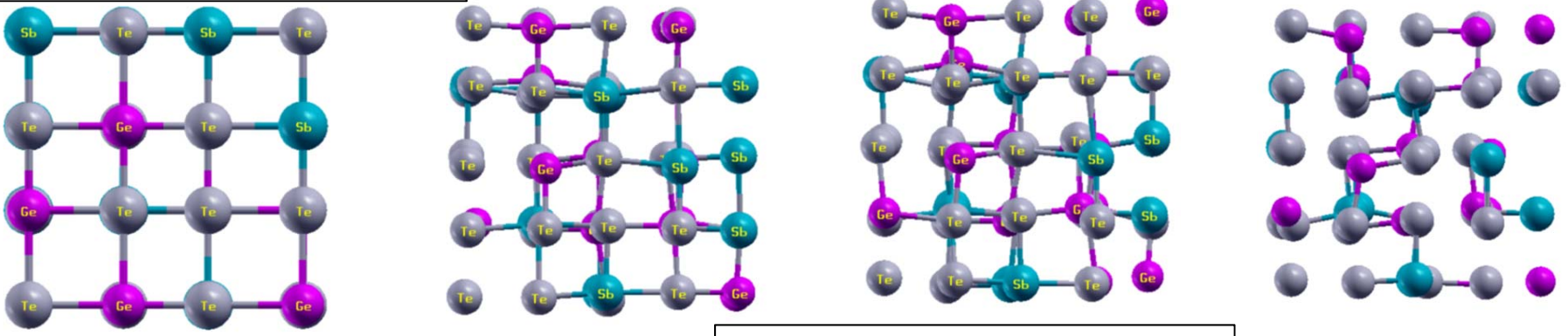
# Piezoelectrically driven Phase Change Memory would be fast, cool & scalable:



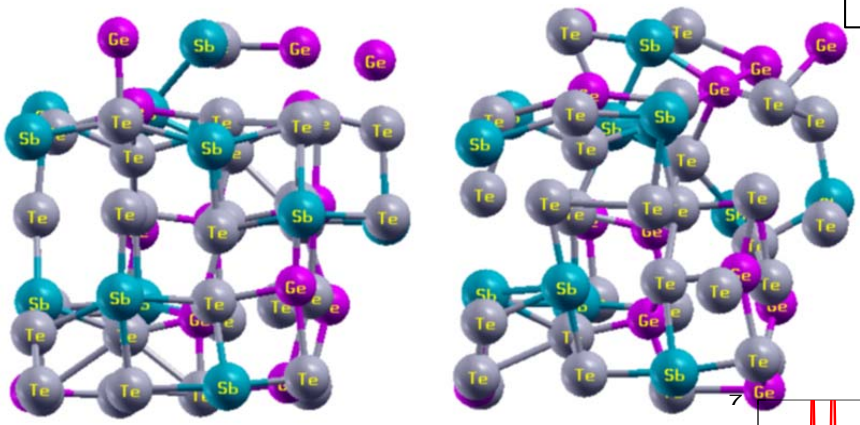

In ON state PCM is in a LOW resistance form → "1".
In OFF state PCM is in a HIGH resistance form → "0".

Can we find suitable material that can be switched by pressure using a combined exp/theor approach?

High Resistance State

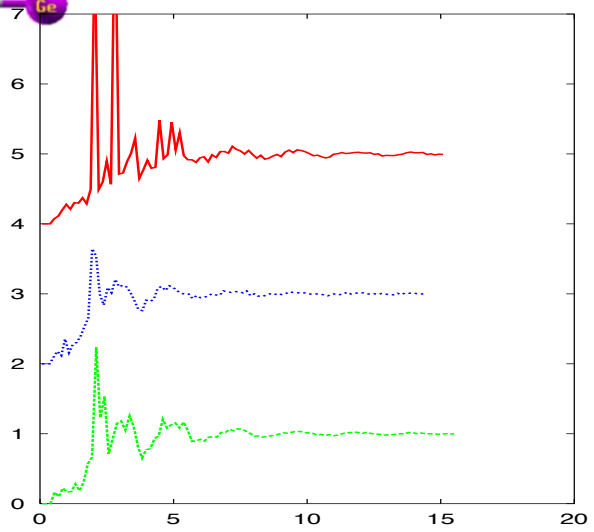


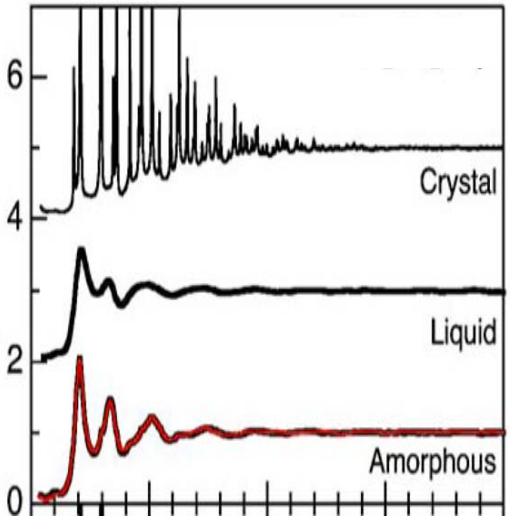
Low Resistance State

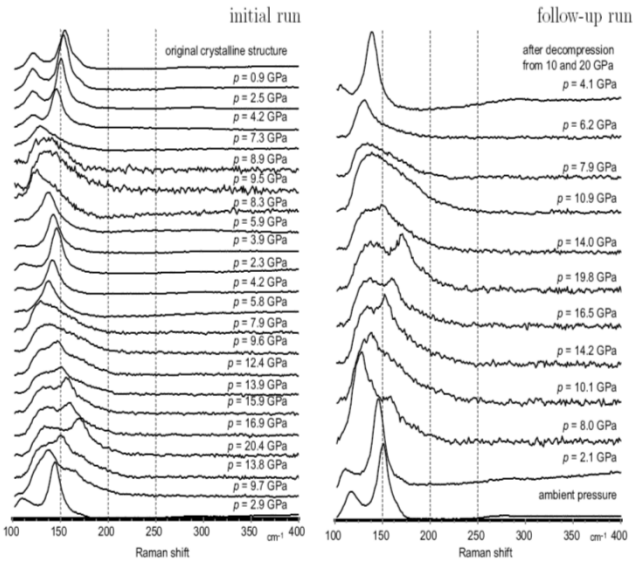


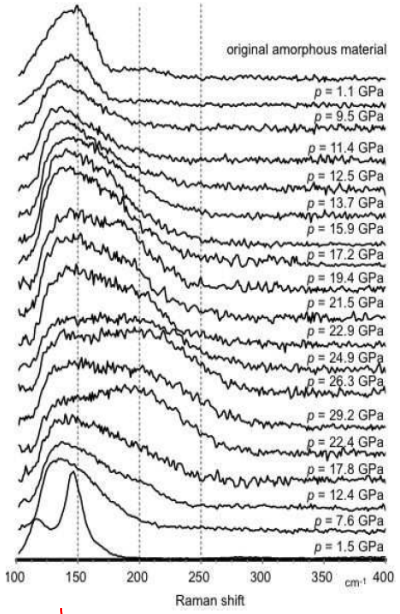
$Ge_2Sb_2Te_5$-undergoes pressure induced "amorphization" both experimentally and theoretically ….

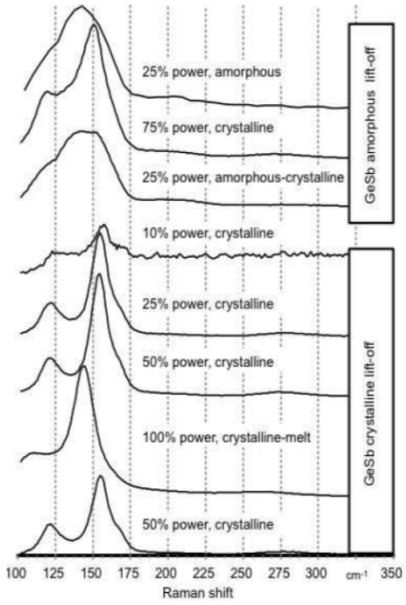
but the process is not reversible!

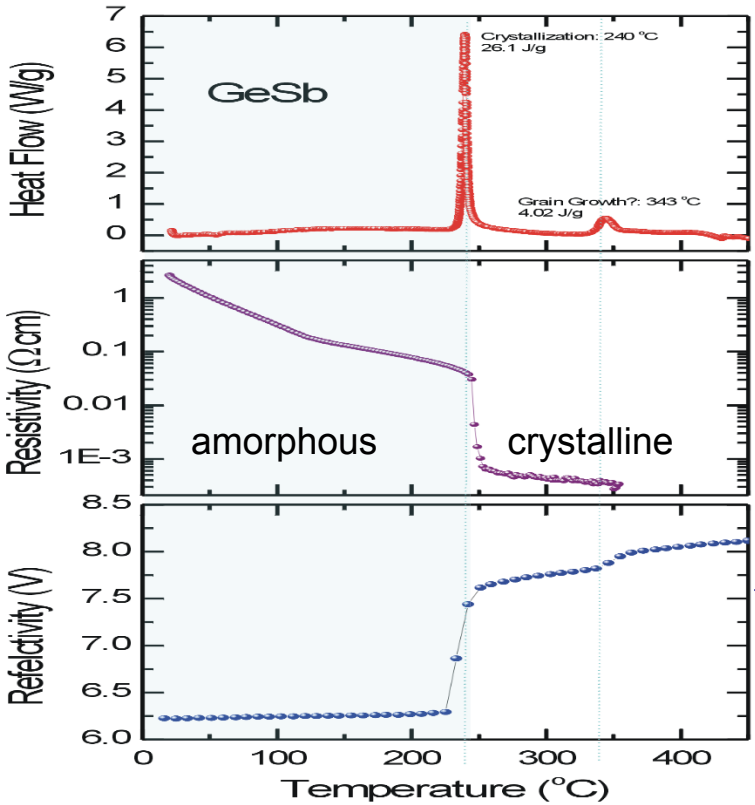




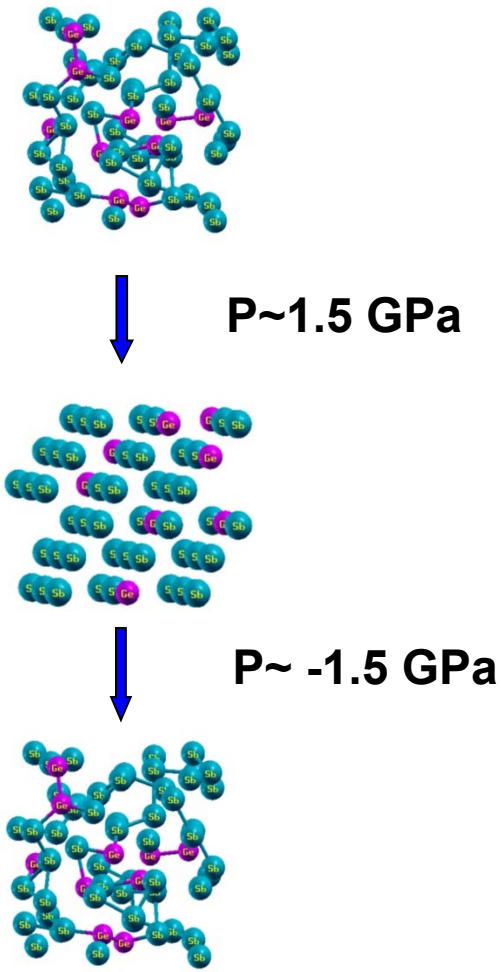




Eutectic GeSb undergoes an amorphous to crystalline transformation under pressure, experimentally!

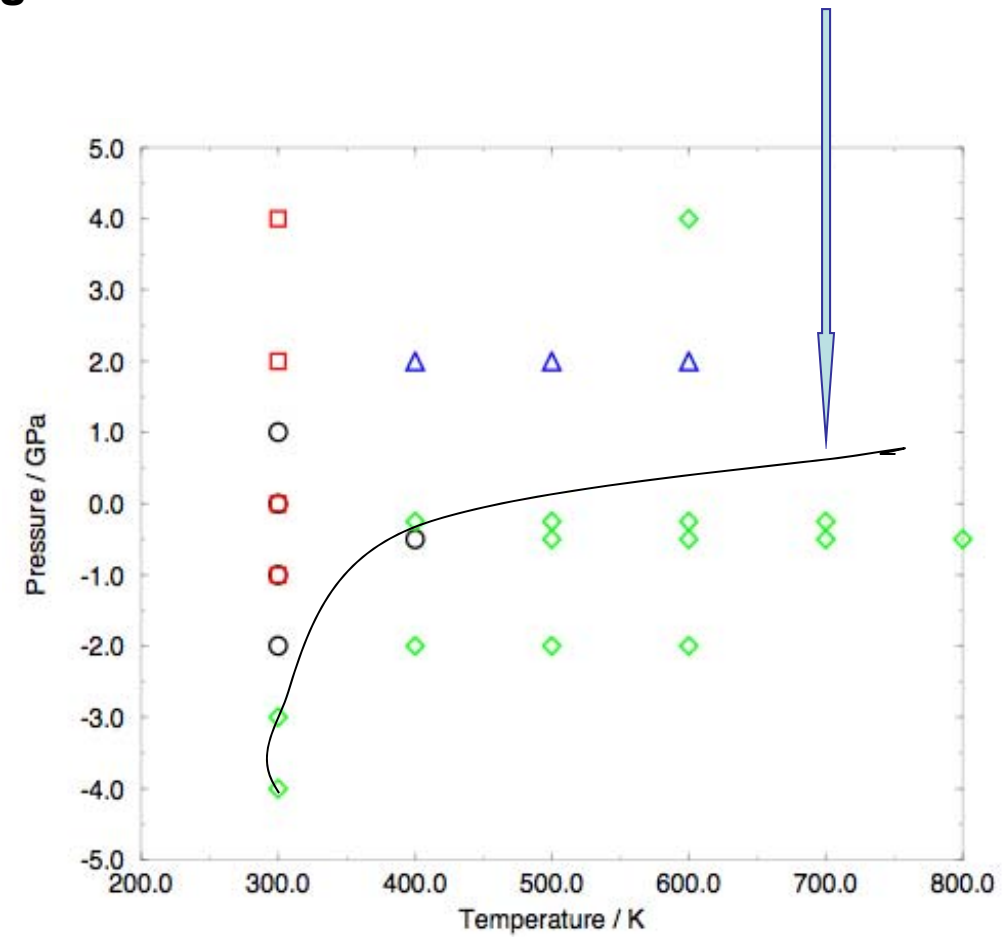
Is the process amenable to reversible switching as in the thermal approach???

# Utilize tensile load to approach the spinodal and cause pressure induced amorphization!

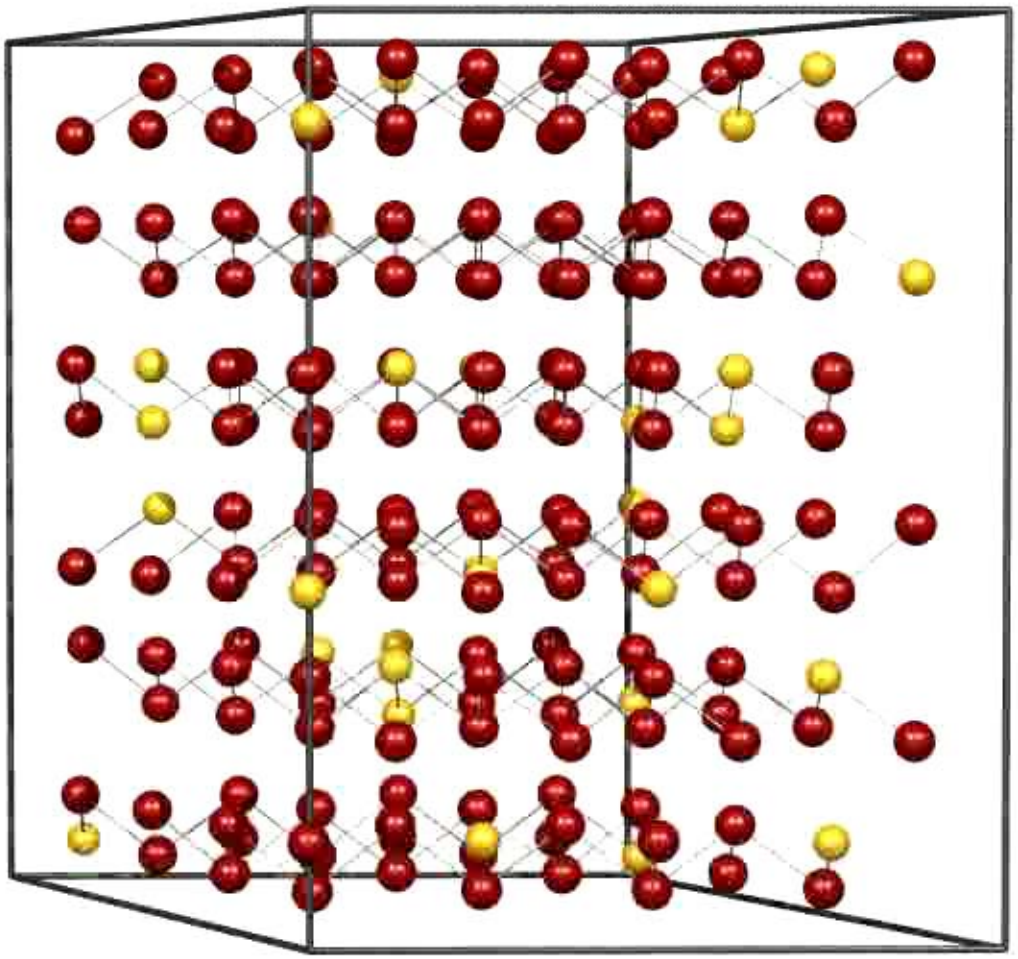
**Schematic of a potential device based on pressure switching**



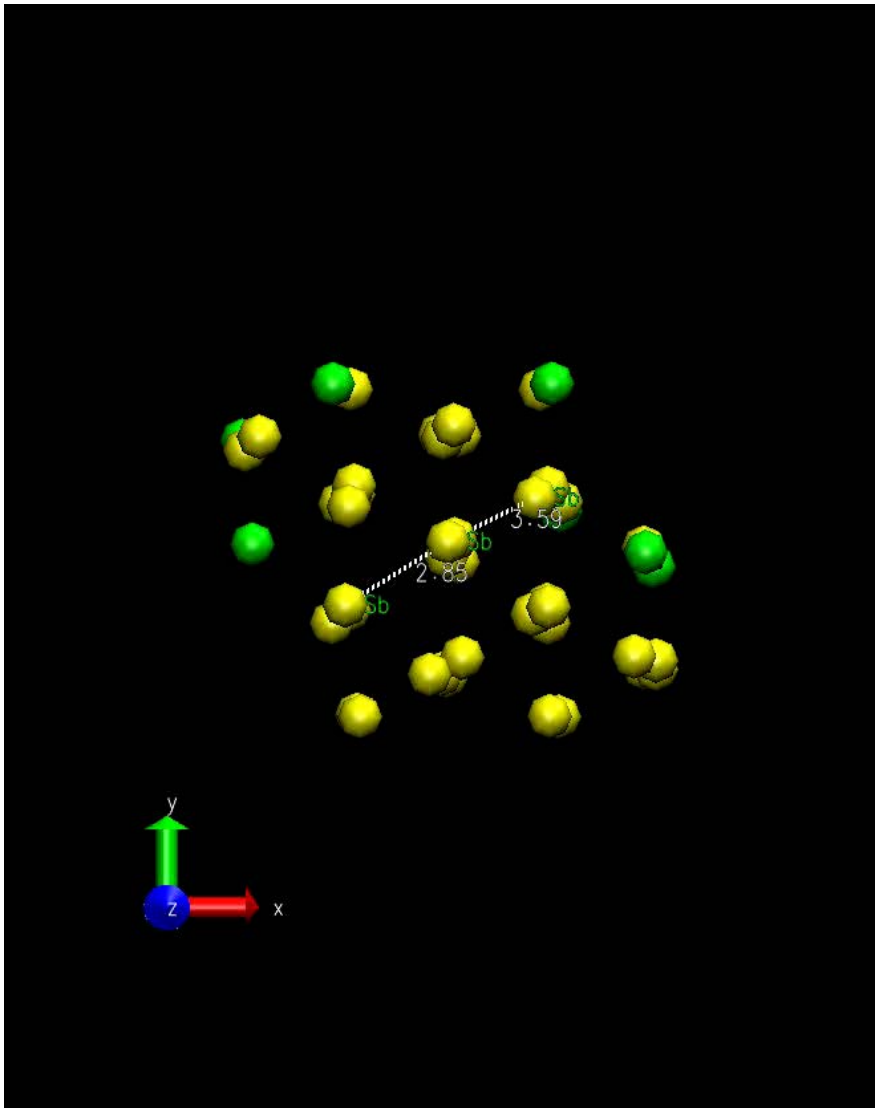

CPAIMD spinodal line!



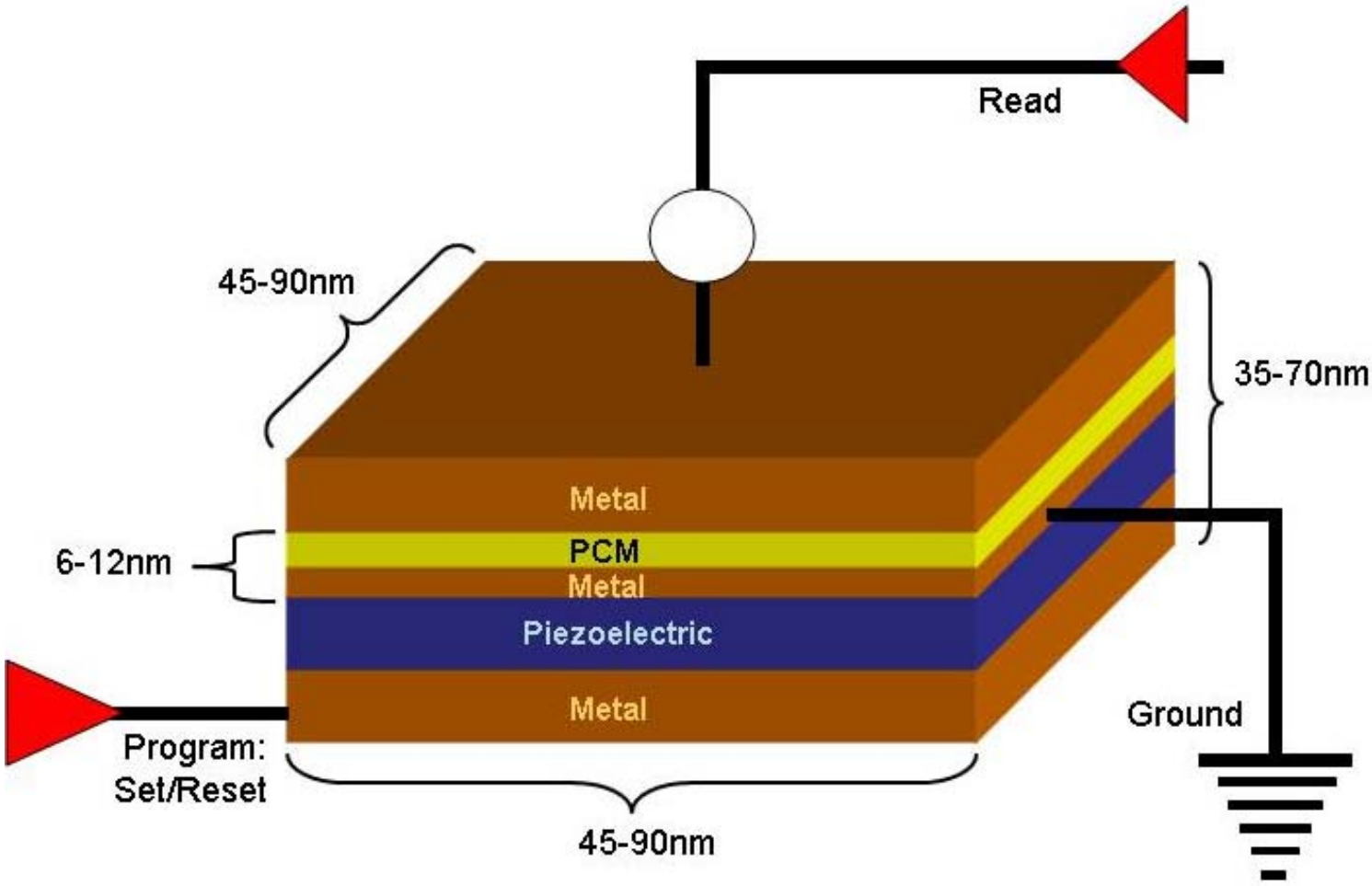
# Spinodal decomposition under tensile load



# Solid is stable at ambient pressure



# IBM's Piezoelectric Memory




We are investigating other materials and better device designs!
Patent filed. Scientific work has appeared in PNAS.

# K-points, Path Integrals and Parallel Tempering

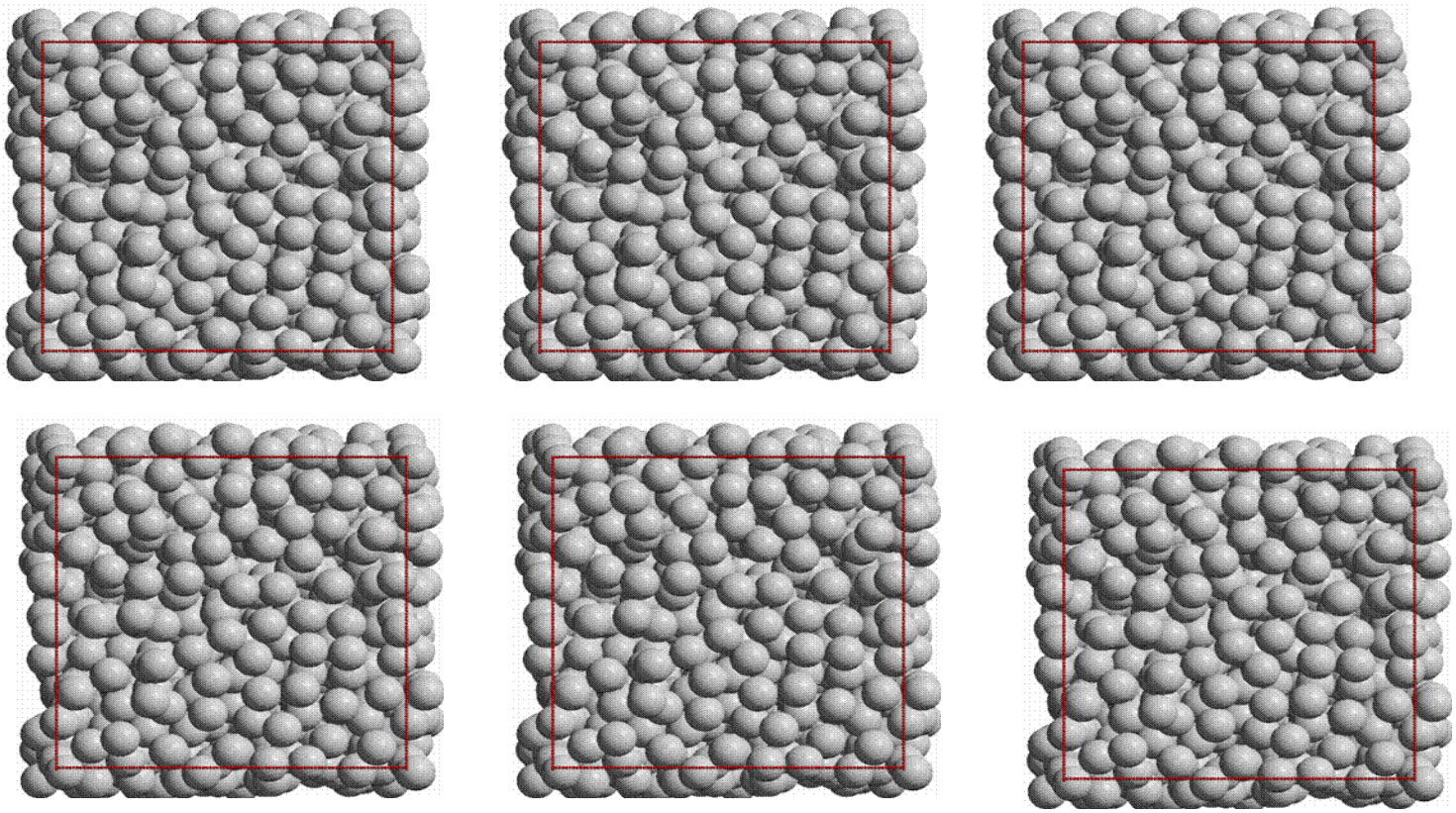
# Instance parallelization

- Many simulation types require fairly uncoupled instances of existing chare arrays.

- Simulation types is this class include:
  1) Path Integral MD (PIMD) for nuclear quantum effects.
  2) k-point sampling for metallic systems.
  3) Spin DFT for magnetic systems.
  4) Replica exchange for improved atomic phase space sampling.

- A full combination of all 4 simulation is both physical and interesting

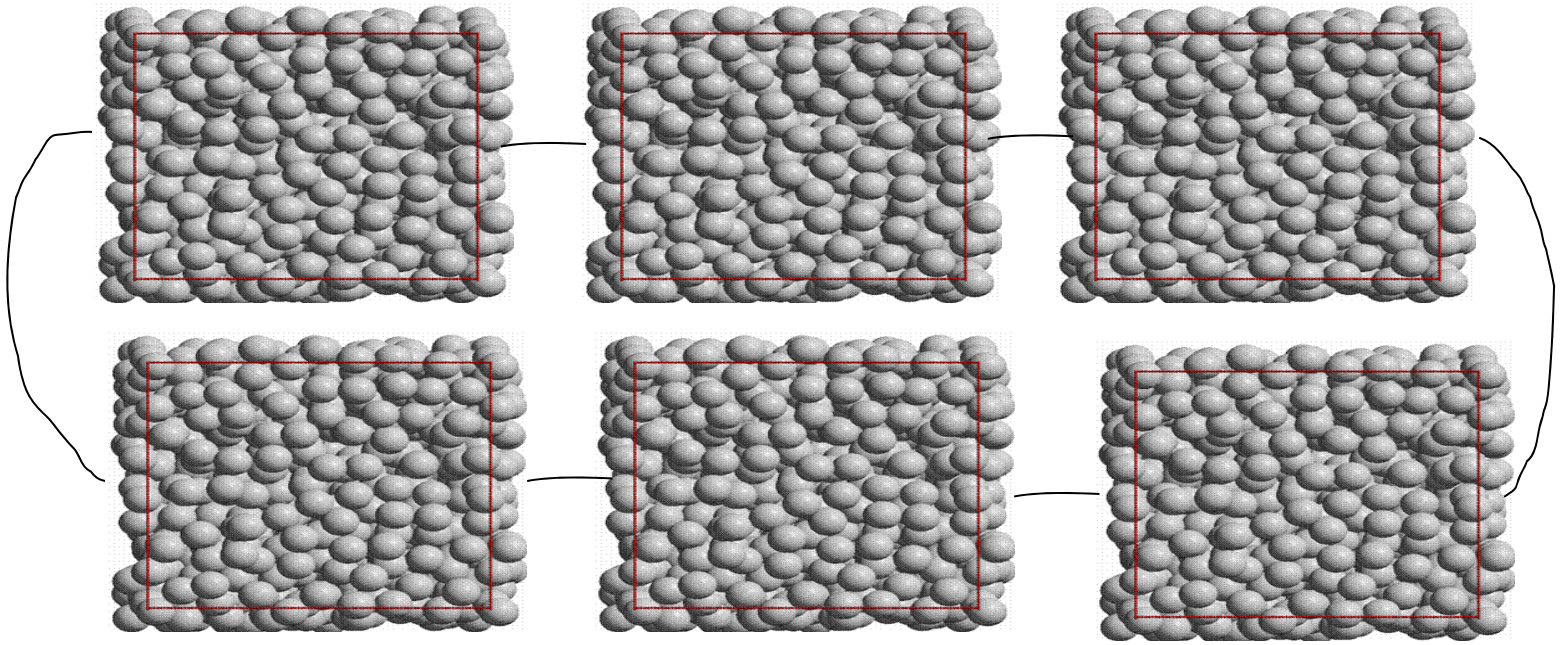
Replica Exchange : M classical subsystems each at a different temperature acting indepently

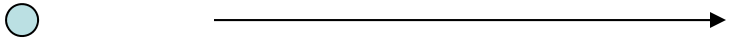


Replica exchange uber index active for all chares.

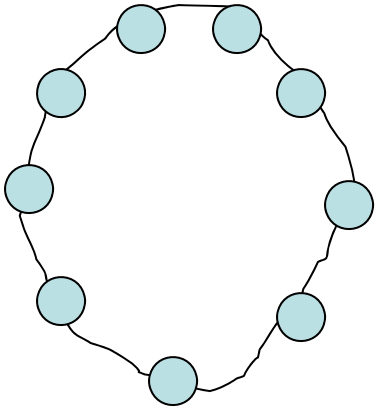
Nearest neighbor communication required to exchange temperatures and energies

# PIMD : P classical subsystems connect by harmonic bonds





Classical particle

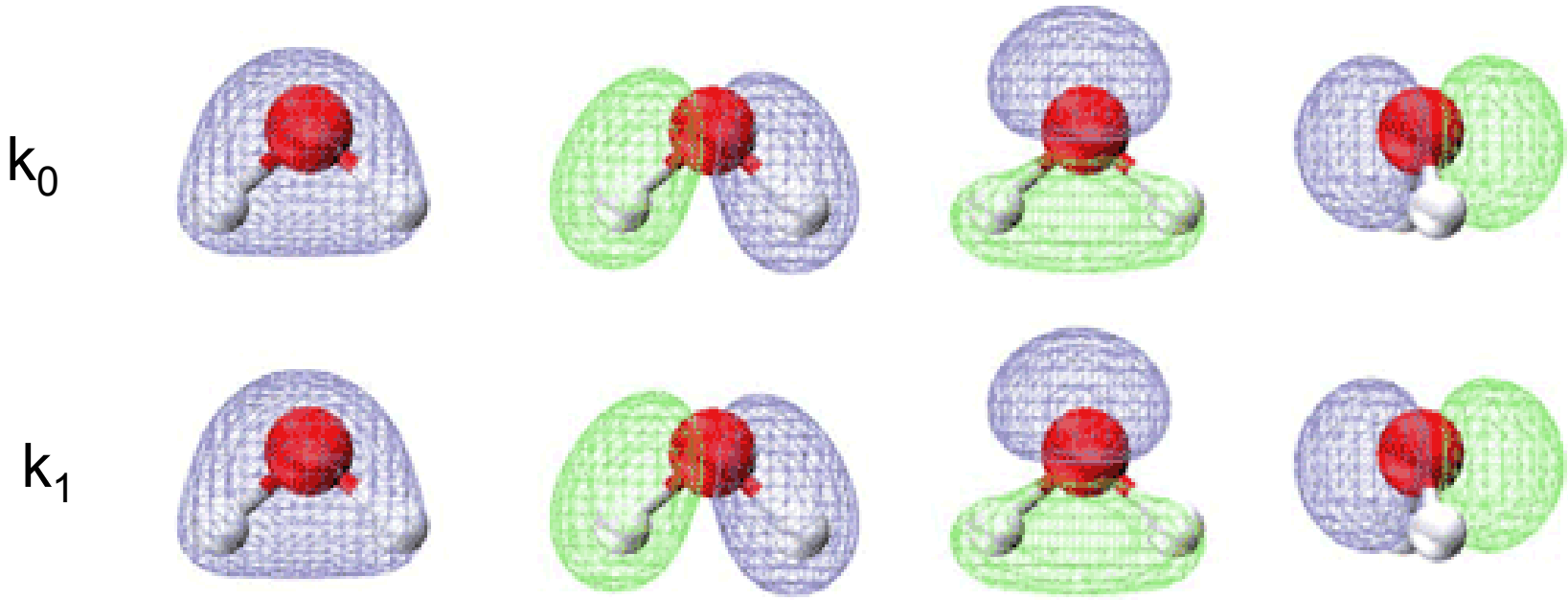


Quantum particle

PIMD uber index active for all chares.

Uber communication required to compute harmonic interactions

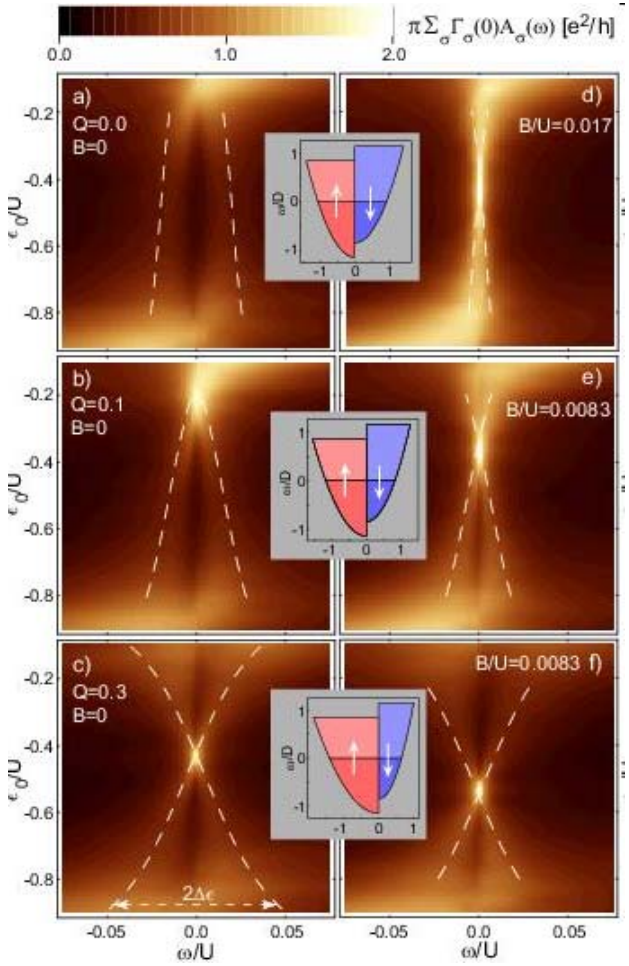
# K-points : N-states are replicated and given a different phase.

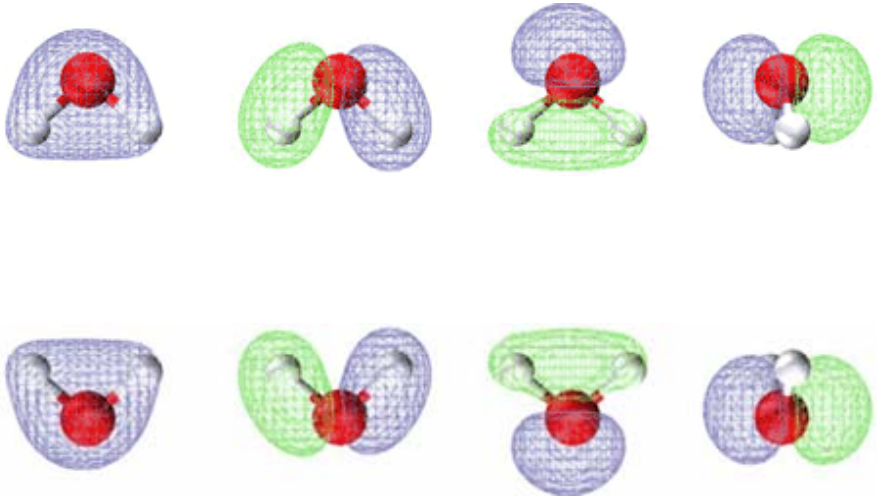



Atoms are assumed to be part of a periodic structure and are shared between the k-points (crystal momenta).

The k-point uber index is not active for atoms and electron density. Uber reduction communication require to form the e-density and atom forces.

# Spin DFT : States and electron density are given a spin-up and spin-down index.



Spin up

Spin dn

The spin uber index is not active for atoms.

Uber reduction communication require to form the atom forces

# ``Uber'' charm++ indices

- Chare arrays in OpenAtom now posses 4 uber ``instance'' indices.
- Appropriate section reductions and broadcasts across the ''Ubers'' have been enabled.
- All physics routines are working.

# Describing exited electrons:

# what, why, how,
# and
# what it has to do with charm++

Sohrab Ismail-Beigi

Applied Physics, Physics, Materials Science
Yale University

# Density Functional Theory

For the ground-state of an interacting electron system

we solve a Schrodinger-like equation for electrons

$$\left[-\frac{\hbar^2\nabla^2}{2m_e} + V_{ion}(r) + \phi(r) + V_{xc}(r)\right]\psi_j(r) = \epsilon_j\,\psi_j(r)$$

Hohenberg & Kohn, Phys. Rev. (1964); Kohn and Sham, Phys. Rev. (1965).

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Tempting: use these electron energies $\epsilon_j$

to describe processes where

electrons change energy
(absorb light, current flow, etc.)

Hohenberg & Kohn, Phys. Rev. (1964); Kohn and Sham, Phys. Rev. (1965).

# DFT: problems with excitations

Energy gaps (eV)

| Material | LDA | Expt. [1] |
|---|---|---|
| Diamond | 3.9 | 5.48 |
| Si | 0.5 | 1.17 |
| LiCl | 6.0 | 9.4 |

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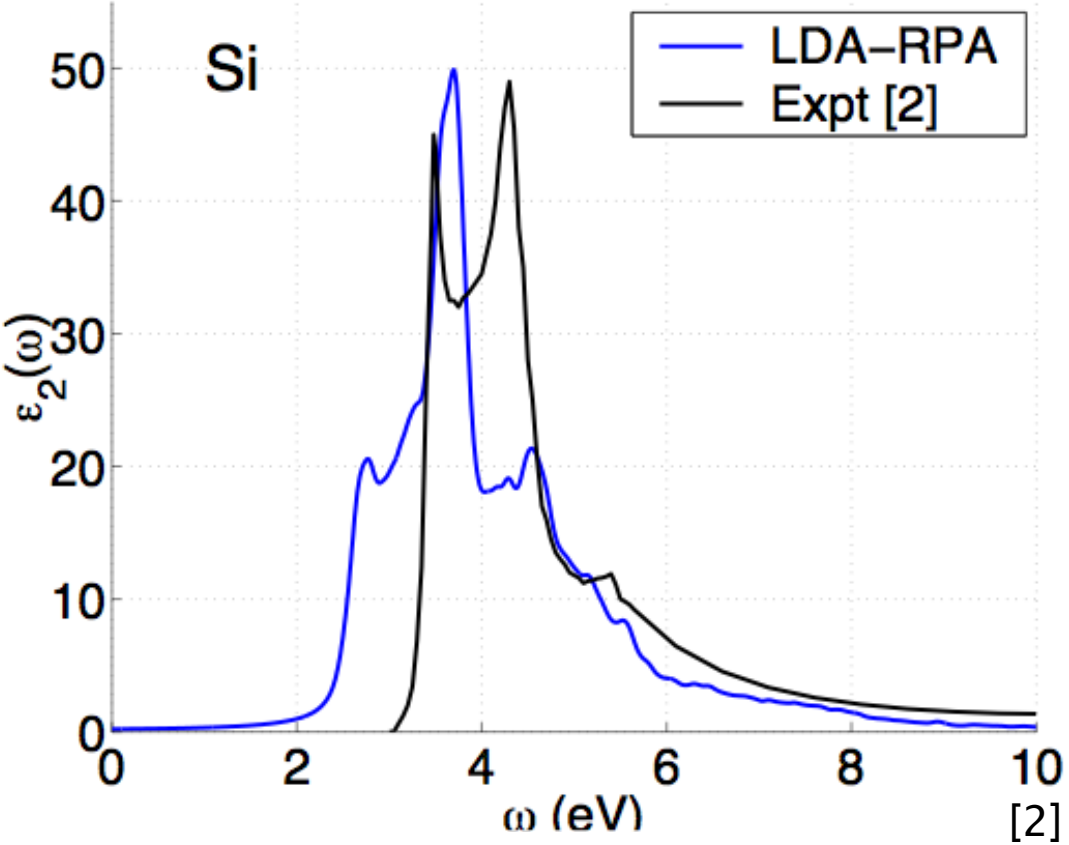


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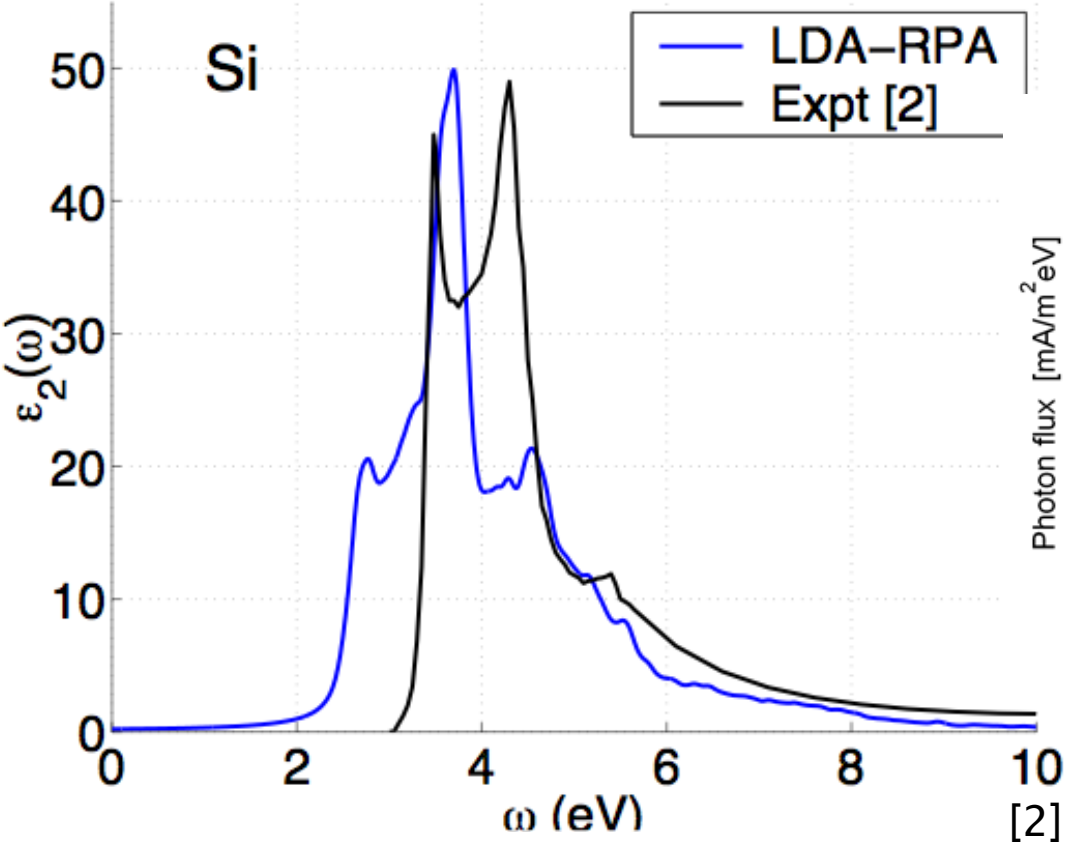
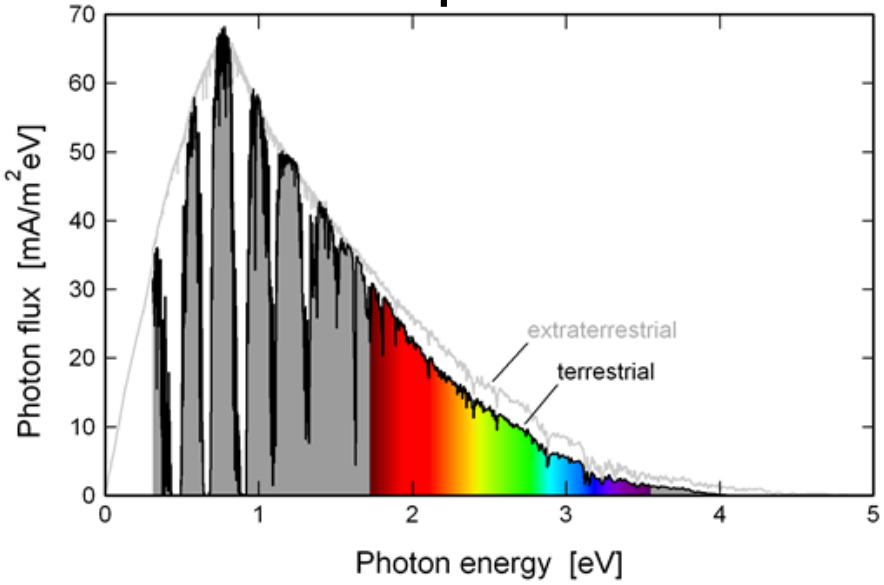



Solar spectrum

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# Green's functions successes

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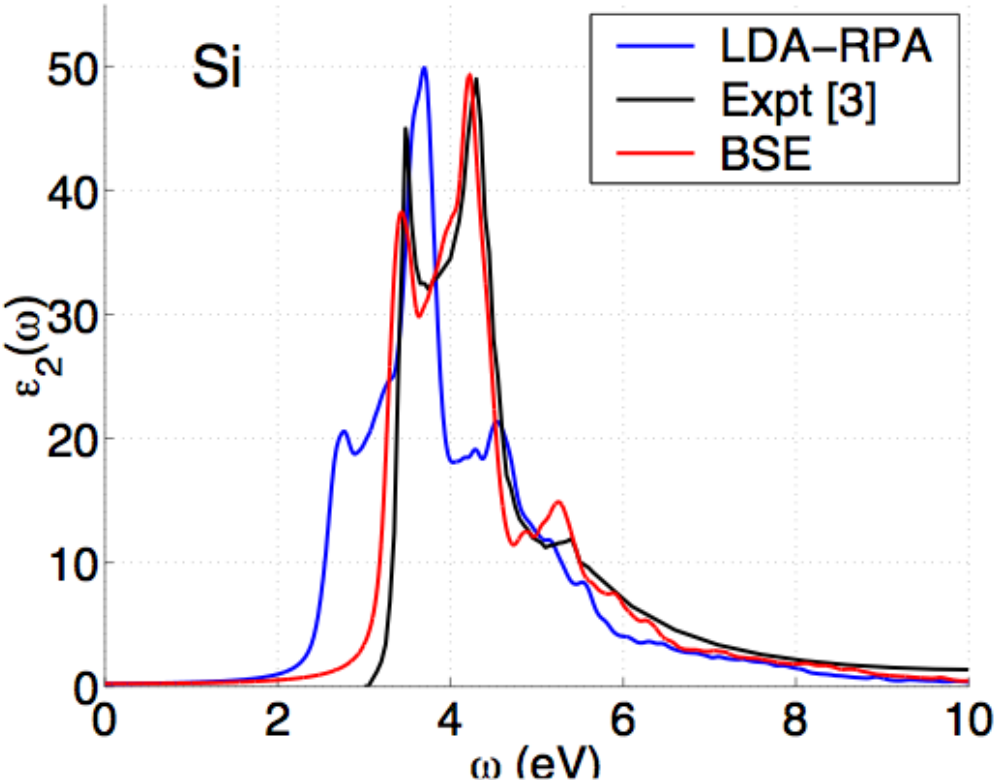

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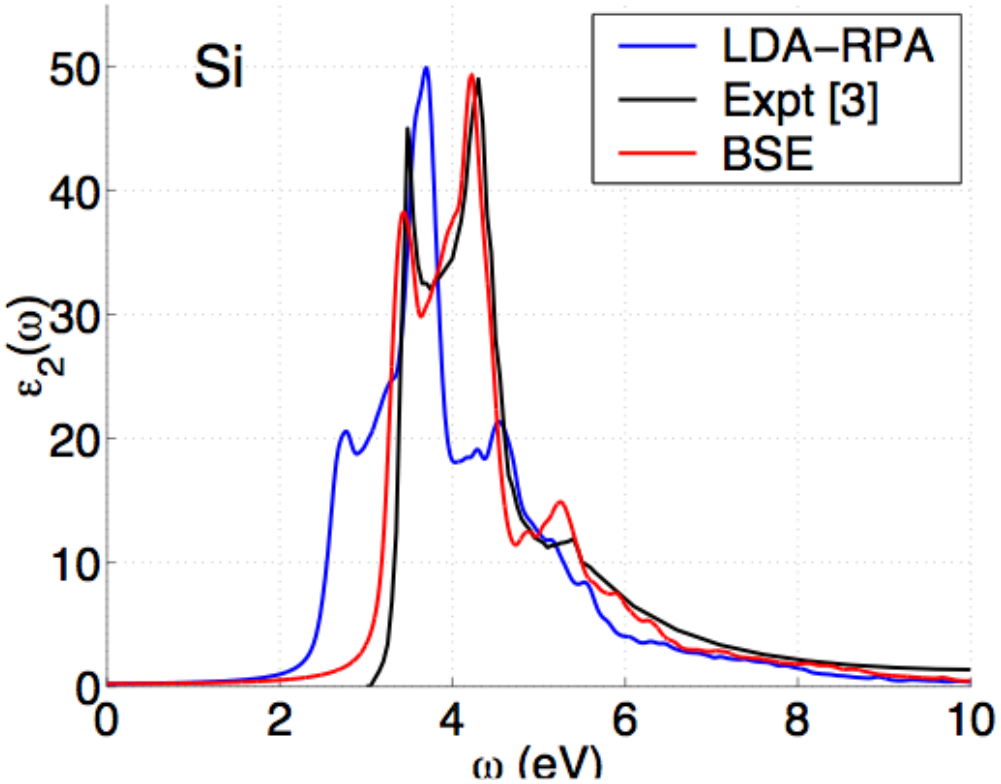


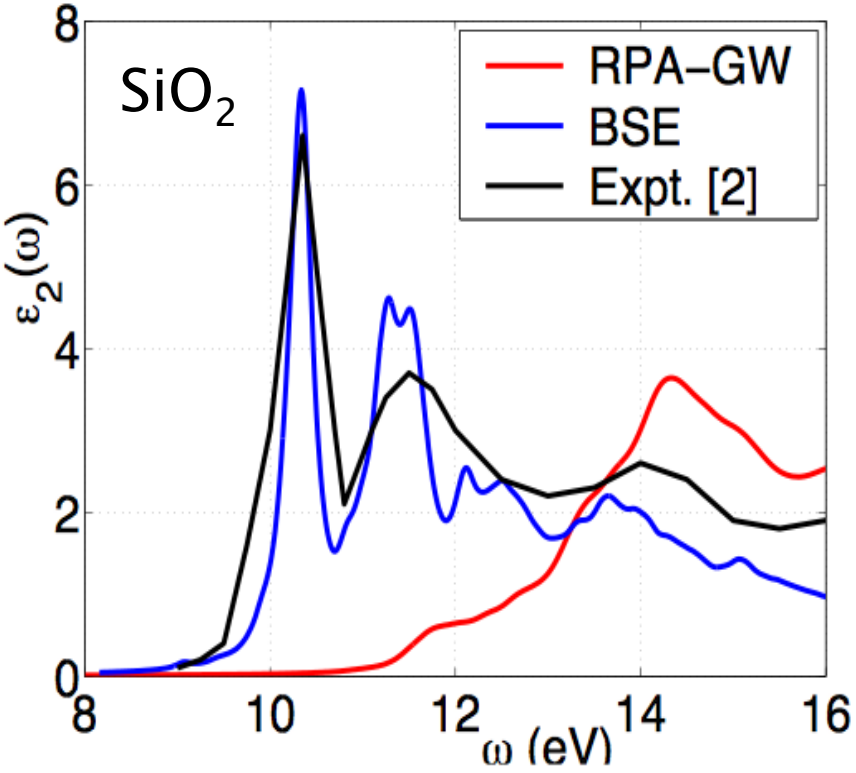

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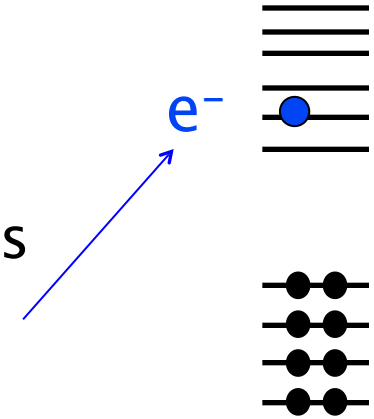

# GW-BSE: what is it about?

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But many processes involve exciting electrons:

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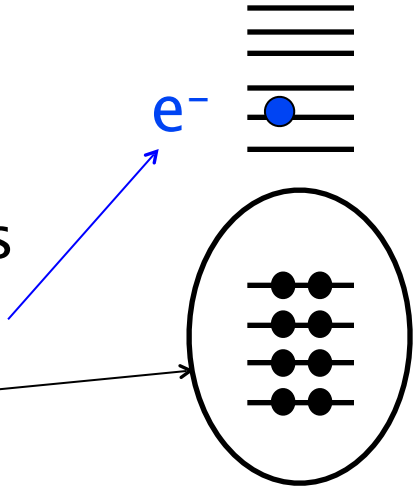
→ The other electrons respond to this and modify energy of added electron



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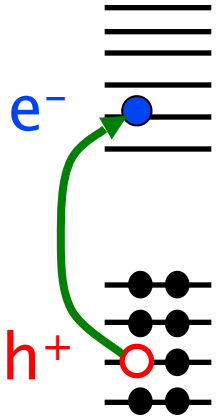
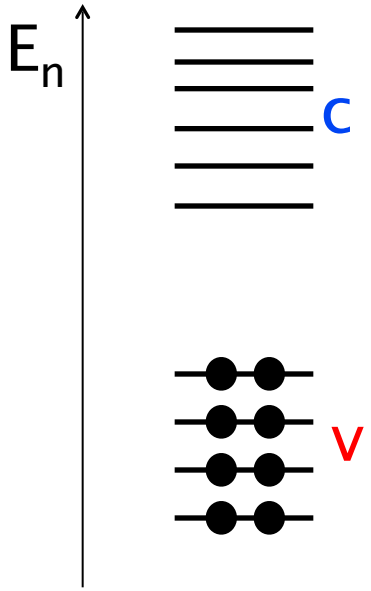


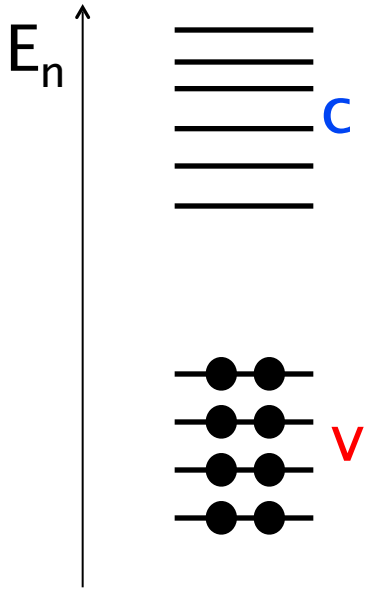
# Optical excitations



# Optical excitations

Single-particle view

- Photon absorbed
- one $e^-$ kicked into an empty state




Problem:

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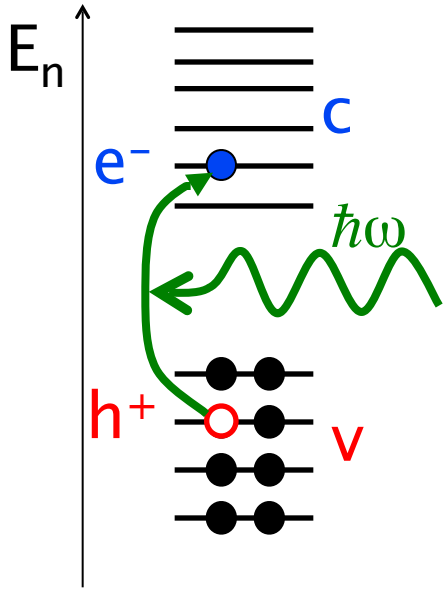


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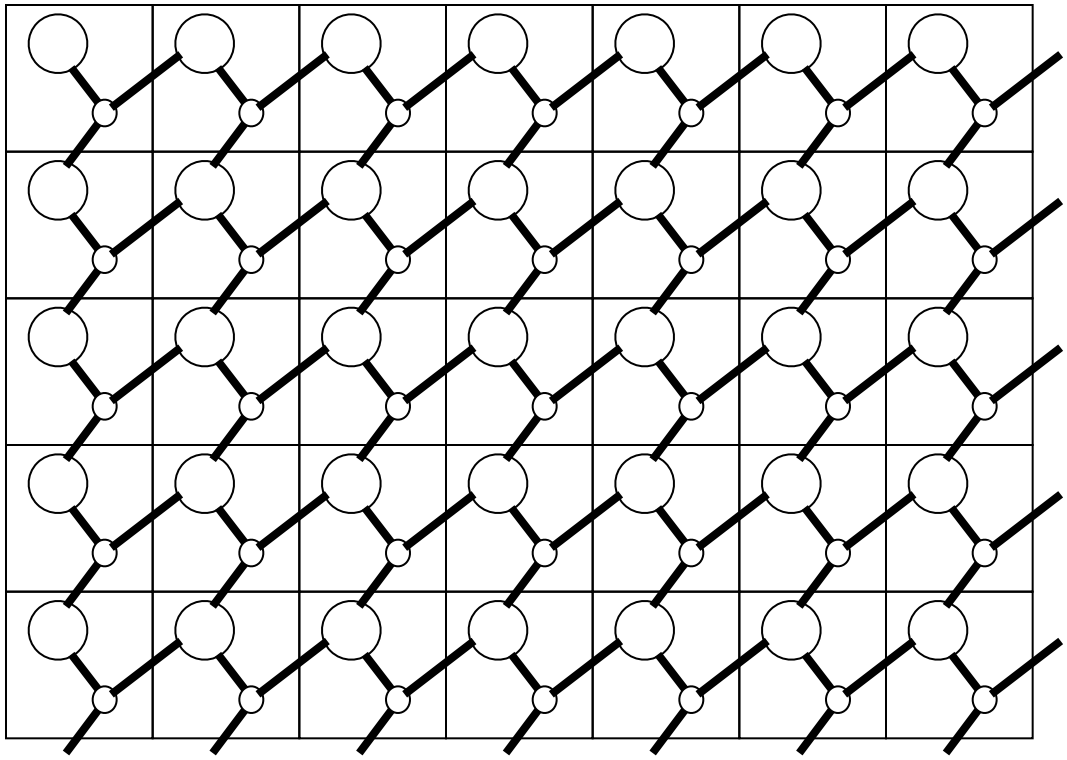
# Optical excitations: excitons

Exciton: correlated $e^-$–$h^+$ pair excitation

Low-energy (bound) excitons: hydrogenic picture



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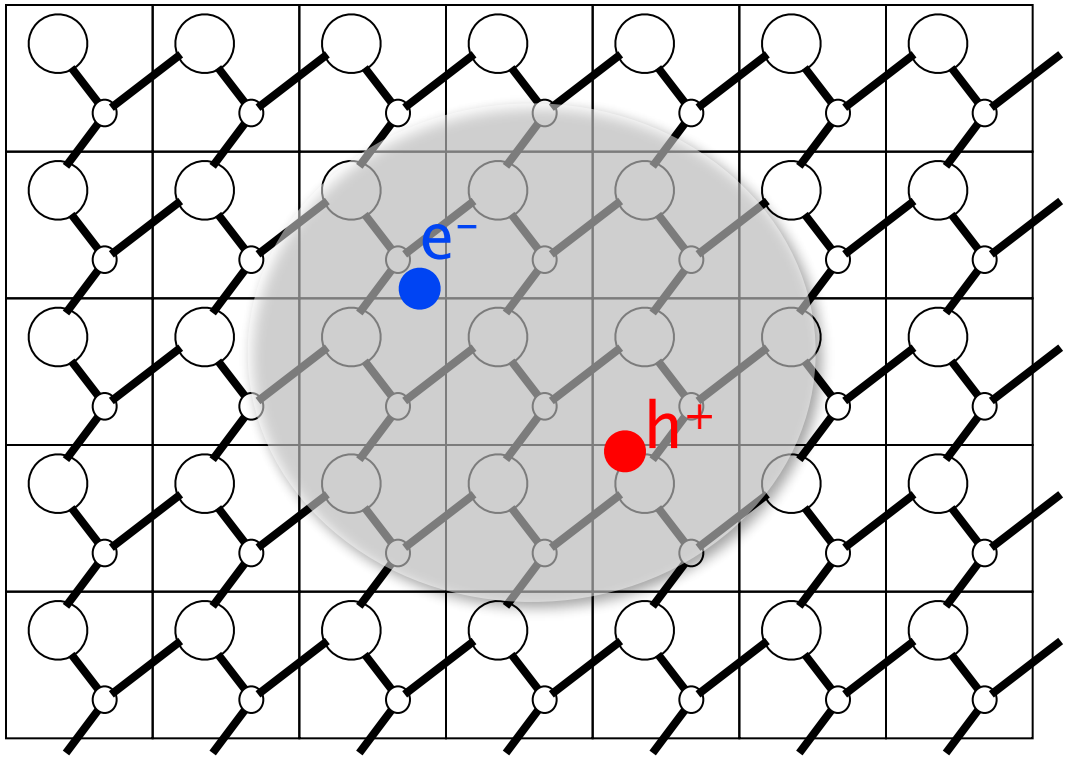

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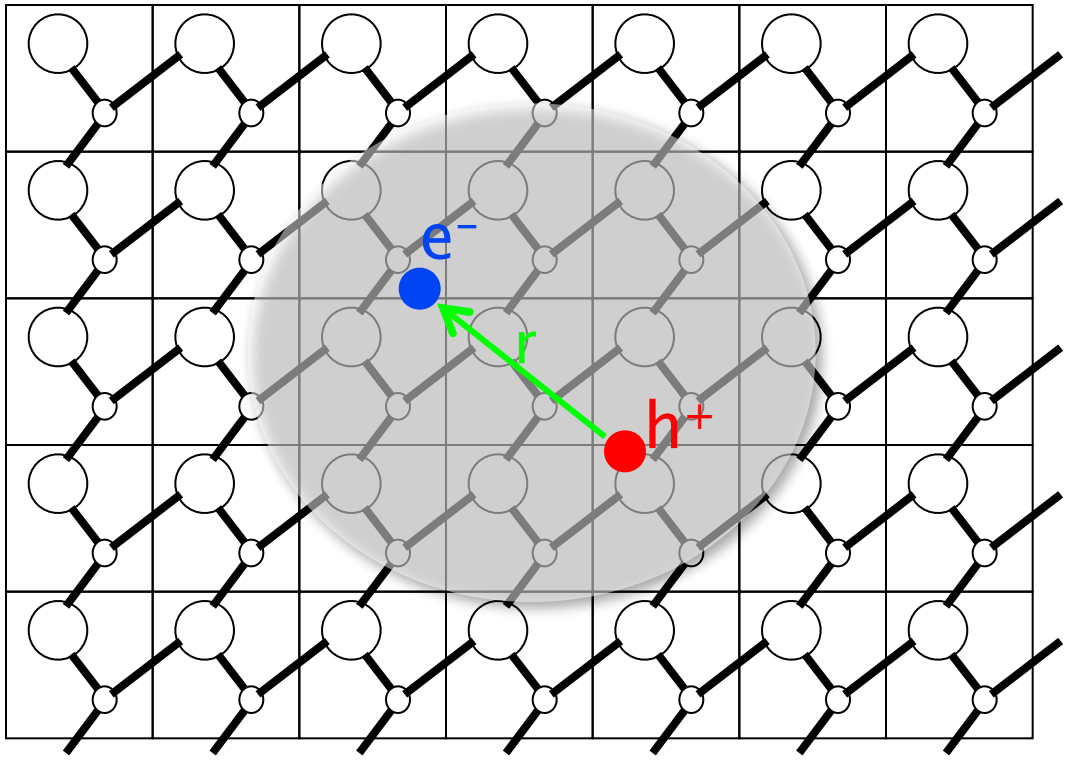

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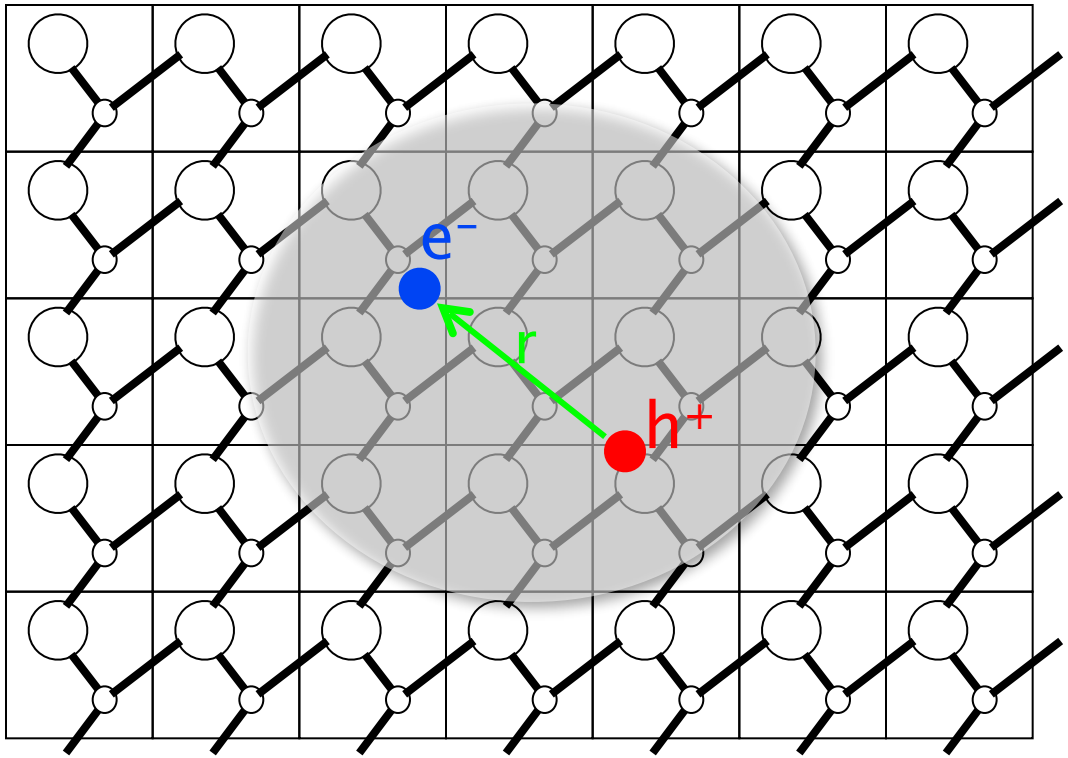


| Material | r (Å) |
|---|---|
| InP | 220 |
| Si | 64 |
| SiO | 4 |

Marder, Condensed Matter Physics (2000)

# GW-BSE: what is it about?

DFT is a ground-state theory for electrons

But many processes involve exciting electrons:

- Transport of electrons

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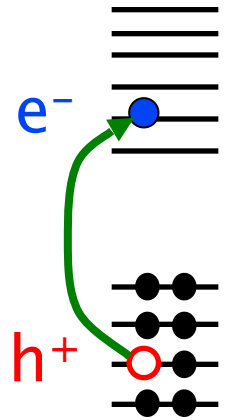


→ The missing electron (hole)
has + charge, attracts electron:
modifies excitation energy and absorption strength

# GW-BSE: what is it about?

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But many processes involve exciting electrons:

- Transport of electrons, electron energy levels
- Excited electrons

Each/both critical in many materials problems, e.g.

- Photovoltaics
- Photochemistry
- “Ordinary” chemistry involving electron transfer

# GW-BSE: what is it for?

DFT is a ground-state theory for electrons

But many processes involve exciting electrons:

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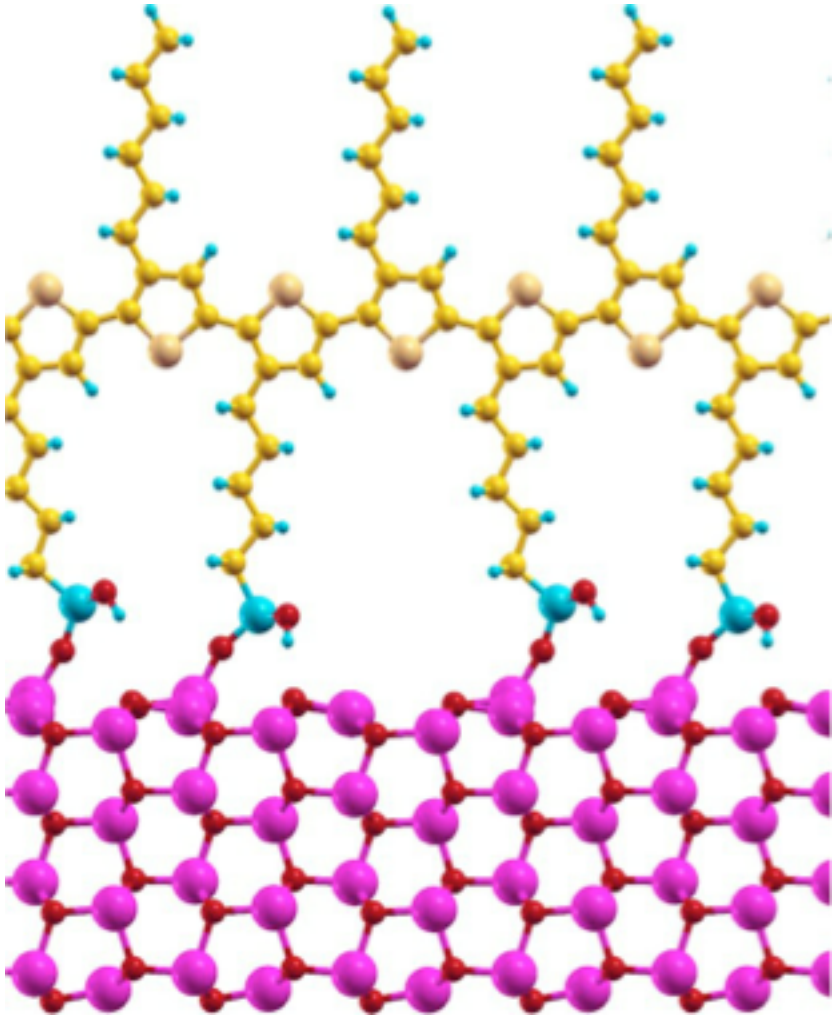
DFT --- in principle and in practice --- does a poor job of describing both

- GW : describe added electron energies
  including response of other electrons
- BSE (Bethe-Salpeter Equation): describe optical processes
  including electron-hole interaction and GW energies

# A system I'd love to do GW-BSE on…

P3HT polymer



Zinc oxide nanowire

But with available GW-BSE methods

it would take "forever"

i.e. use up all my supercomputer allocation time

# GW-BSE is expensive

Scaling with number of atoms N

- DFT : $N^3$
- GW : $N^4$
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e.g. a system with 50-75 atoms (GaN)

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Hence, our first focus is on GW

Once that is scaling well, we will attack the BSE

# What's in the GW?

Key element : compute response of electrons to perturbation

$$P(r,r') = \frac{\partial n(r)}{\partial V(r')} = \sum_{i}^{\text{filled}} \sum_{j}^{\text{empty}} \frac{\psi_i(r)\psi_j(r)\psi_i(r')\psi_j(r')}{\epsilon_i - \epsilon_j}$$

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Challenges

1. Many FFTs to get wave functions $\psi_i(r)$ functions
2. Large outer product to form $P$
3. Dense $r$ grid : $P(r,r')$ is huge in memory
4. Sum over $j$ is very large

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1 & 2 : Efficient parallel FFTs and linear algebra
3 : Effective memory parallelization
4 : replace explicit $j$ sum by implicit inversion

# Summary

GW-BSE is promising as it contains the right physics

Very expensive : computation and memory

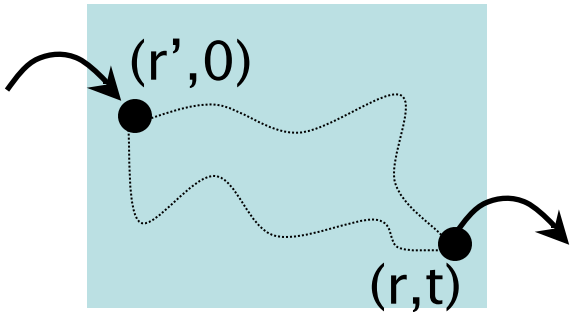
Plan to implement high performance version in
OpenAtom for the community (SI2-SSI NSF grant)

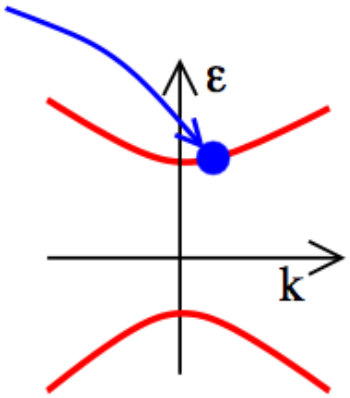
Two sets of challenges

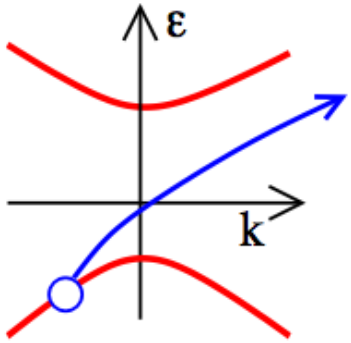
- How to best parallelize existing GW-BSE algorithms?
  Will rely on Charm++ to deliver high performance
  Coding, maintenance, migration to other computers
  much easier for user

- Need to improve GW-BSE algorithms to use the computers
  more effective (theoretical physicist/chemist's job)

# One particle Green's function




$$G_1(r,r',\omega) = \sum_j \frac{\psi_j(r)\psi_j(r')^*}{\omega - \epsilon_j}$$

Dyson Equation:

$$\left[-\frac{\nabla^2}{2} + V_{ion}(r) + V_H(r) + \Sigma(r,r',\epsilon_j)\right]\psi_j(r) = \epsilon_j\psi_j(r)$$

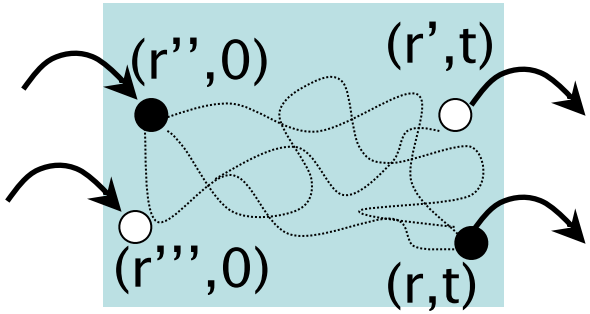
$$\Sigma \approx iG_1W \quad , \quad W = \varepsilon^{-1}(\omega) * v_c \quad (RPA)$$

DFT:

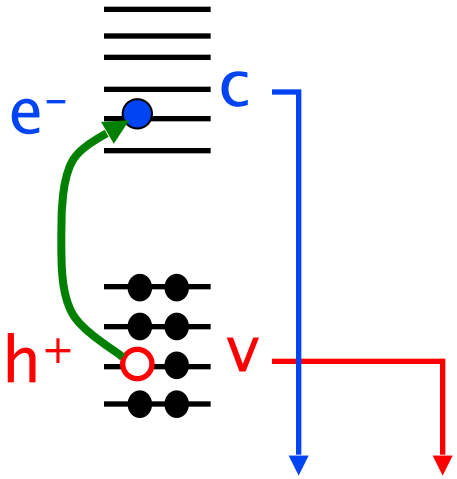
$$\left[-\frac{\nabla^2}{2} + V_{ion}(r) + V_H(r) + V_{xc}(r)\right]\psi_j(r) = \epsilon_j\psi_j(r)$$

Hedin, Phys. Rev. (1965); Hybertsen & Louie, Phys. Rev. B (1986).

# Two particle Green's function




$$G_2(\omega) = \sum_S \frac{\Phi_S \cdot \Phi_S^*}{\omega - \Omega_S}$$




Exciton amplitude:

Bethe-Salpeter Equation: $H A^S = \Omega_S A^S$
(BSE)

$$H = \epsilon_c - \epsilon_v + K_{int}$$

$$\langle K_{int} \rangle = -\int dr \int dr' \, |\Phi_S(r,r')|^2 \, W(r,r')$$

attractive
(screened direct)

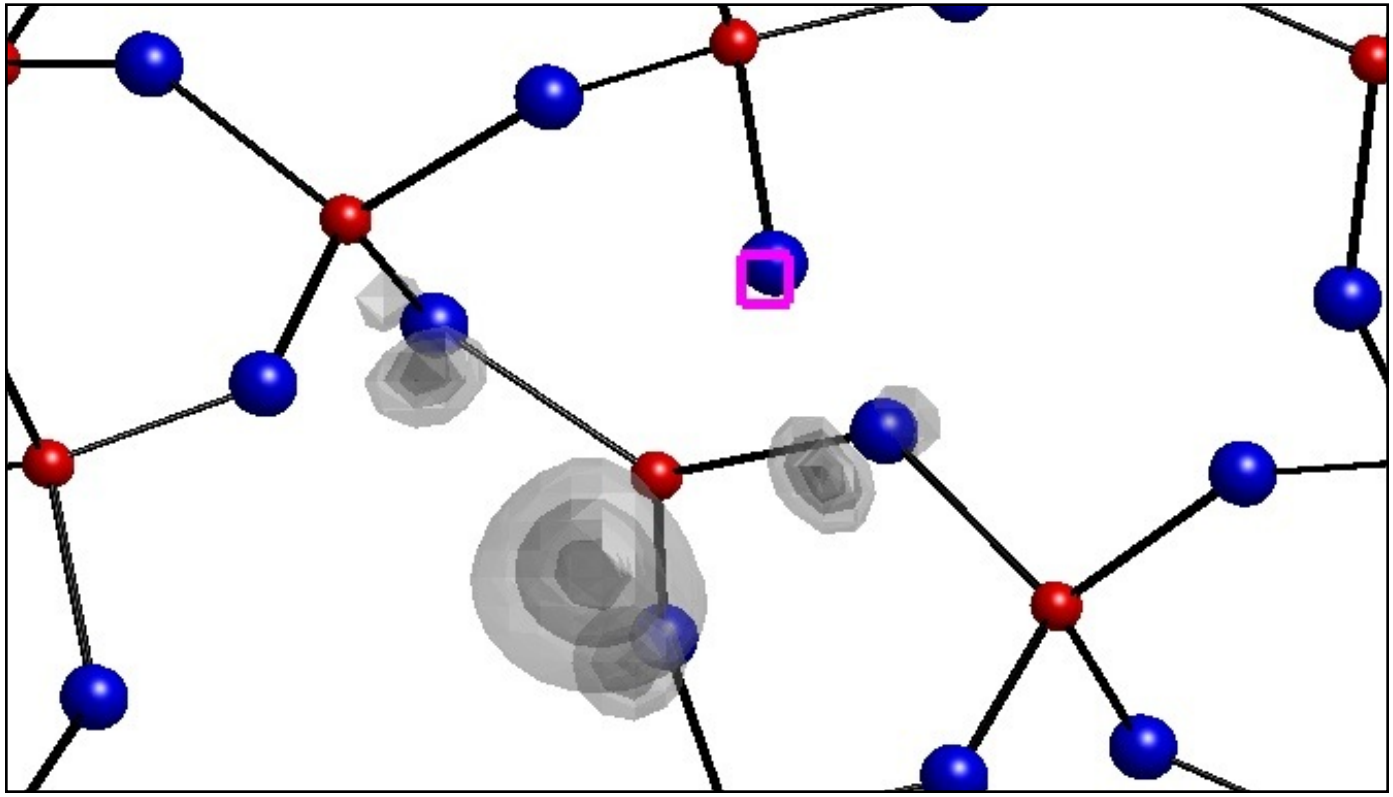
$$+ \int dr \int dr' \, \Phi_S^*(r,r) \Phi_S(r',r') \, v_c(r-r')$$

repulsive
(exchange)

Rohlfing & Louie; Albrecht et al.; Benedict et al.: PRL (1998)

# STE geometry

Prob : 20,40,60,80% max



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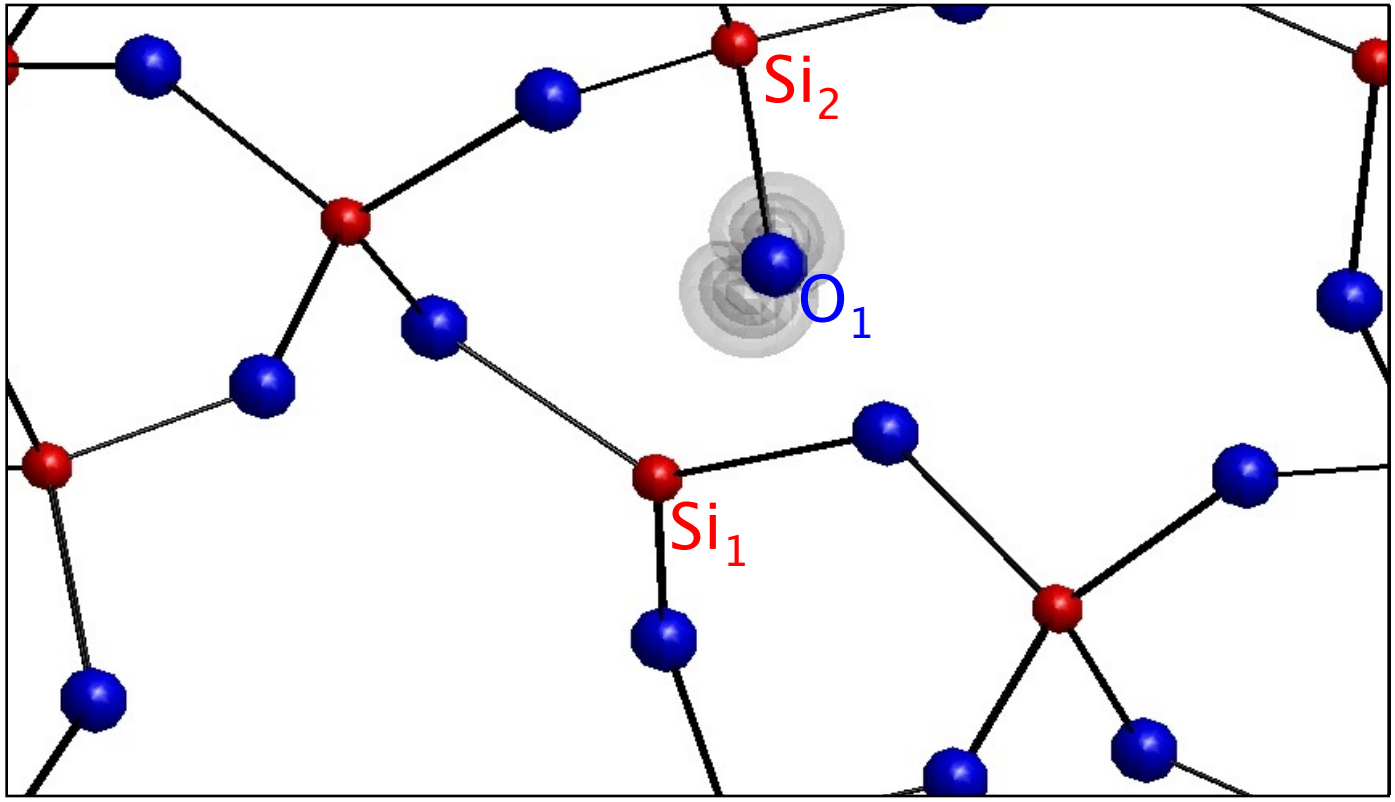

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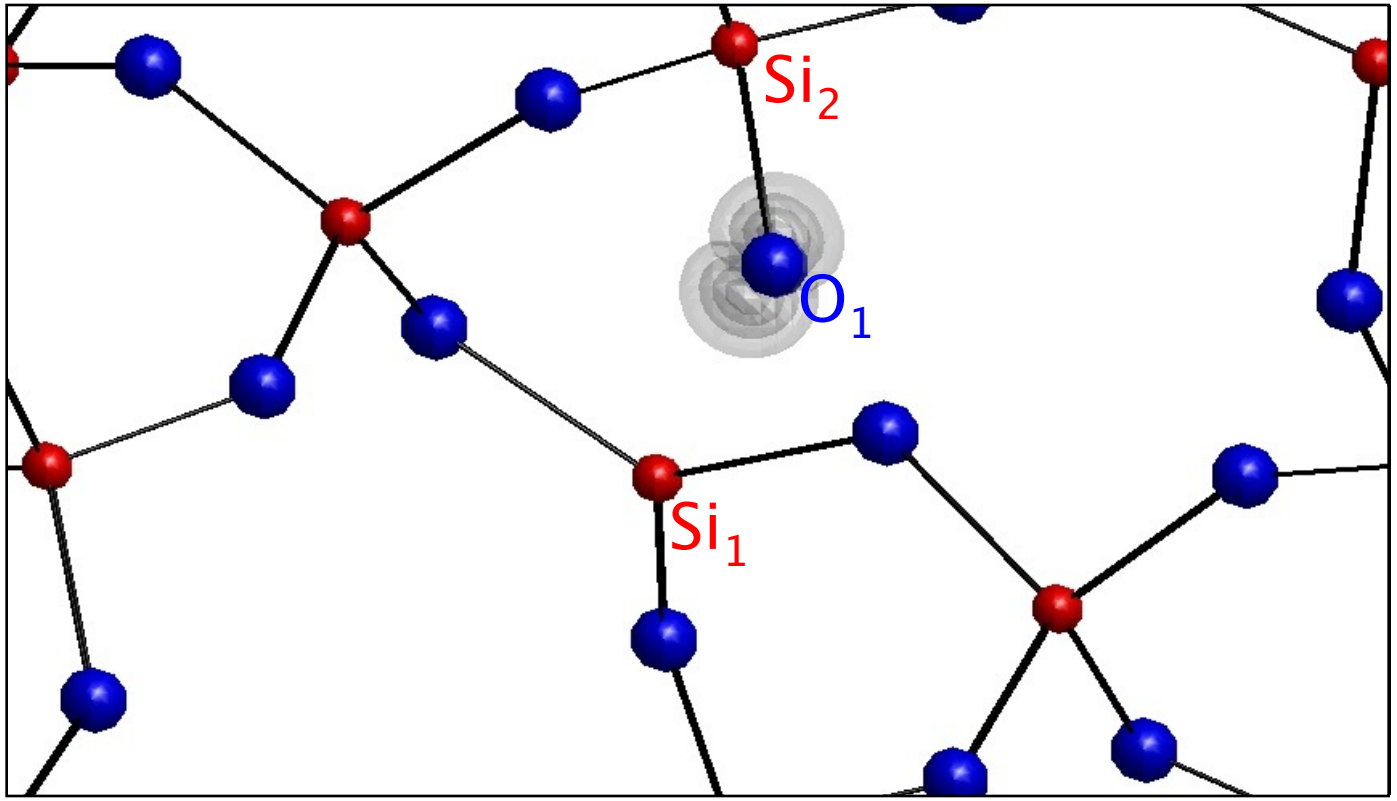


| Bond (Å) | Bulk | STE |
|---|---|---|
| Si | 1.60 | 1.97 (+23%) |
| Si | 1.60 | 1.68 (+5%) |
| Si | 1.60 | 1.66 (+4%) |

| Angles | Bulk | STE |
|---|---|---|
| O | 109 | ≈ 85 |
| O | 109 | ≈ 120 |

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Defects → localized states: exciton can get trapped

Interesting case: self-trapping

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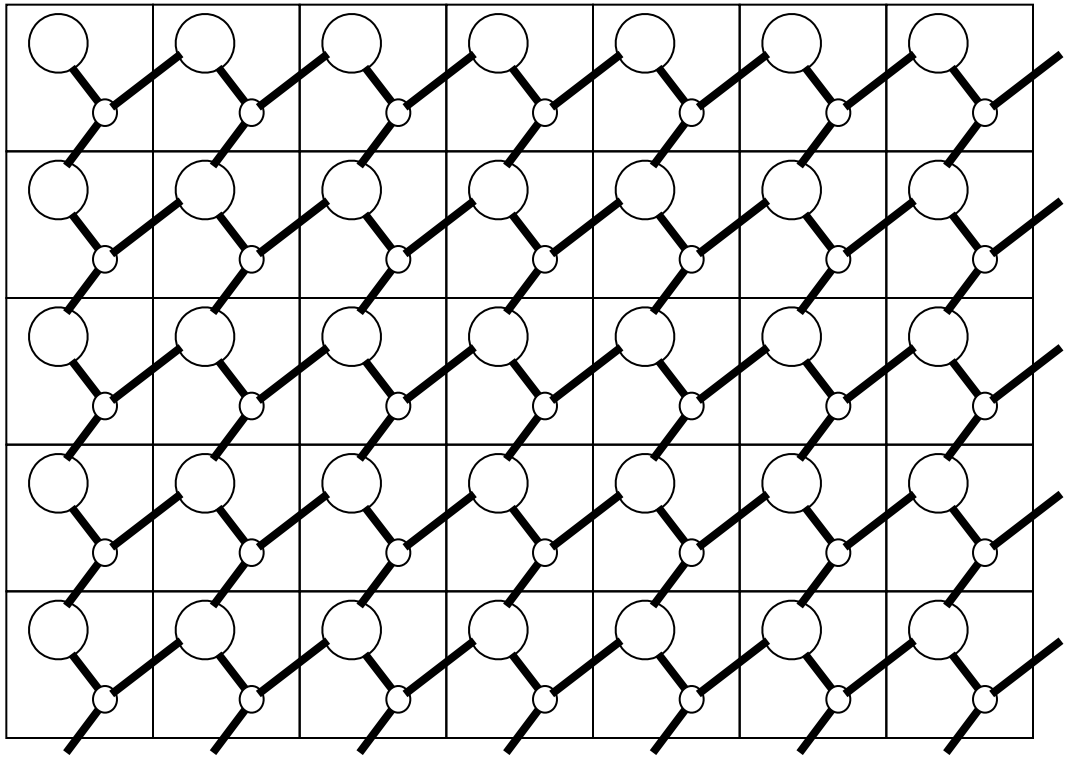

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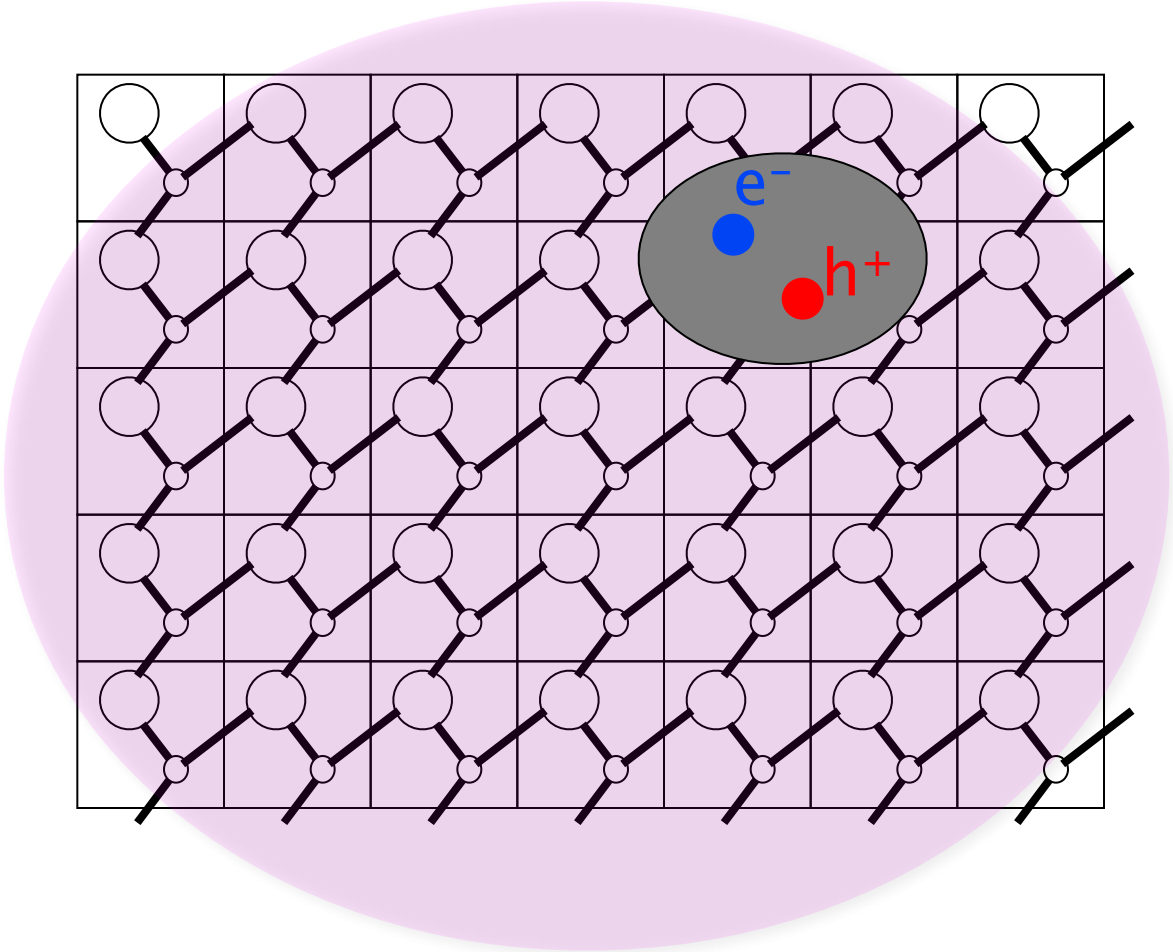

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