



High Performance Computing on Condensed Matter Physics

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Condensed Matter Physics

- Condensed phases: **solids** and **liquids**.
- Condensed matter physics deals with the macroscopic/microscopic physical properties of condensed matters.



Physical properties of Condensed Matter

- **Macroscopic physical properties:** Phonon spectrum; heat capacity; hardness; superconductivity; magnetism; Raman and Infrared spectra; thermoelectricity; bulk modulus; optical and near edge absorption spectra, etc.
- **Microscopic physical properties:** Crystal structure; growth and phase transition mechanisms, etc.

Is numerical simulation necessary?

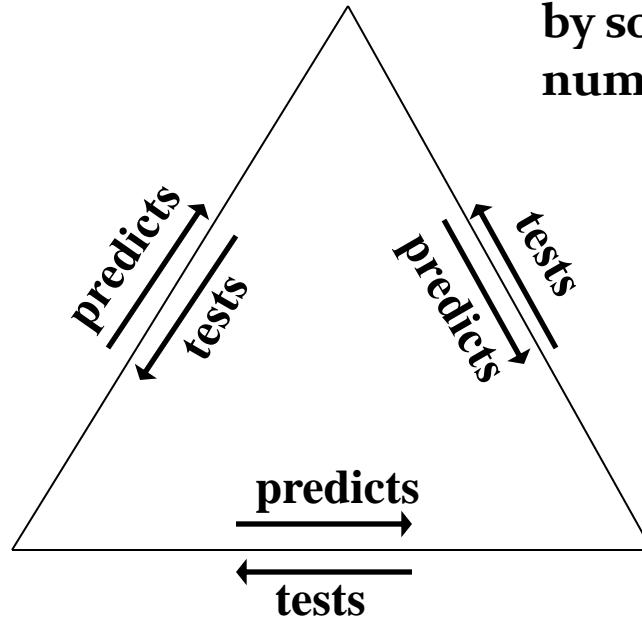
- ⦿ Experiments have limitations under certain circumstances (e.g., samples, techniques, signals, etc) so that many physical properties can not be measured accurately.
- ⦿ Microscopic process (e.g., growth and phase transition mechanism, etc) of understanding the physics are not experimentally measurable.

Numerical computation must be relied on

Computational Physics

Computation

Performs idealized "experiments" on the computer by solving physical models numerically



Theory

Construction of idealized models through mathematical (analytical) analysis of physical principle to describe nature

Experiments

Quantitative measurement of physical properties

Simulation methods

Classical – described by classical (Newtonian) mechanics.

Quantum – described by the Schrödinger equation (or its analogues).

Quantum electronic effects – exchange-correlation, anti symmetry of the wave function, Heisenberg uncertainty principle, electronic kinetic energy. ALWAYS IMPORTANT!

Quantum effects in atomic motion – 1) zero-point energy, 2) Heat capacity and thermal expansion go to zero at $T = 0$ K. IMPORTANT ONLY AT LOW TEMPERATURES.

Atomistic methods – electrons are not considered. Instead, INTERATOMIC interactions, parameterised by some functions, are used.

Simulation methods

° Semiempirical methods – simplified quantum-mechanical treatments (some effects neglected, some approximated).

Hartree-Fock – exact exchange, neglect of correlation.

Density functional theory – in principle exact, in practice approximate for both exchange and correlation.

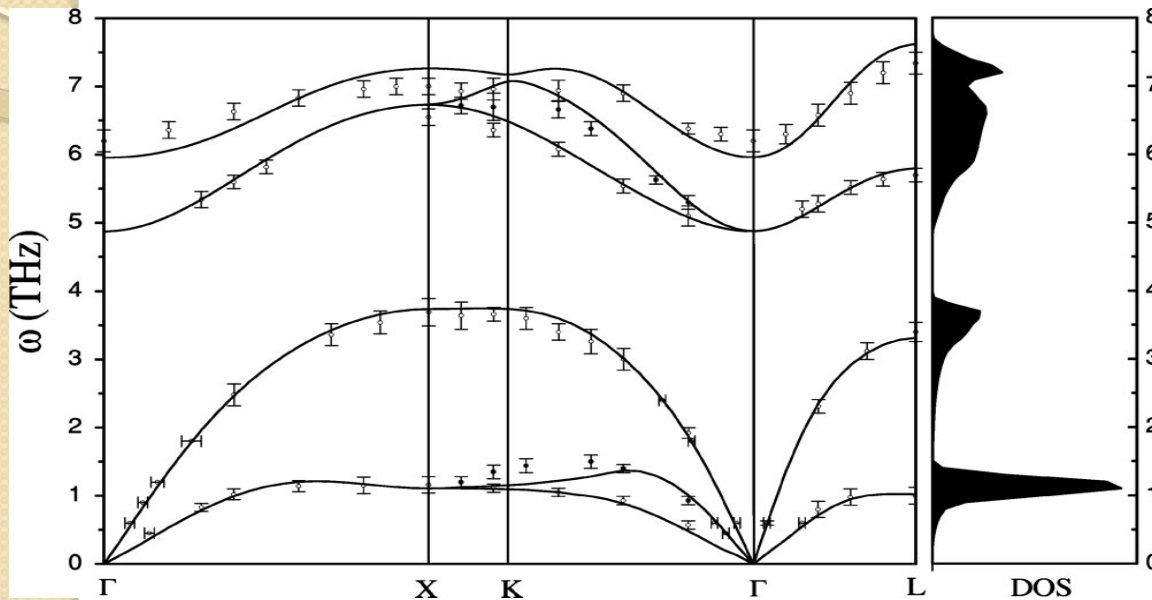
Quantum Monte Carlo – nearly exact method with a stochastic procedure for finding the many-body wave function.

Computer "experiments"

- ◉ **With the development of computer science and computation physics, many properties of matters can be accurately predicted by theoretical simulations.**
- ◉ **The computational physics can be called as “computer experiments”.**



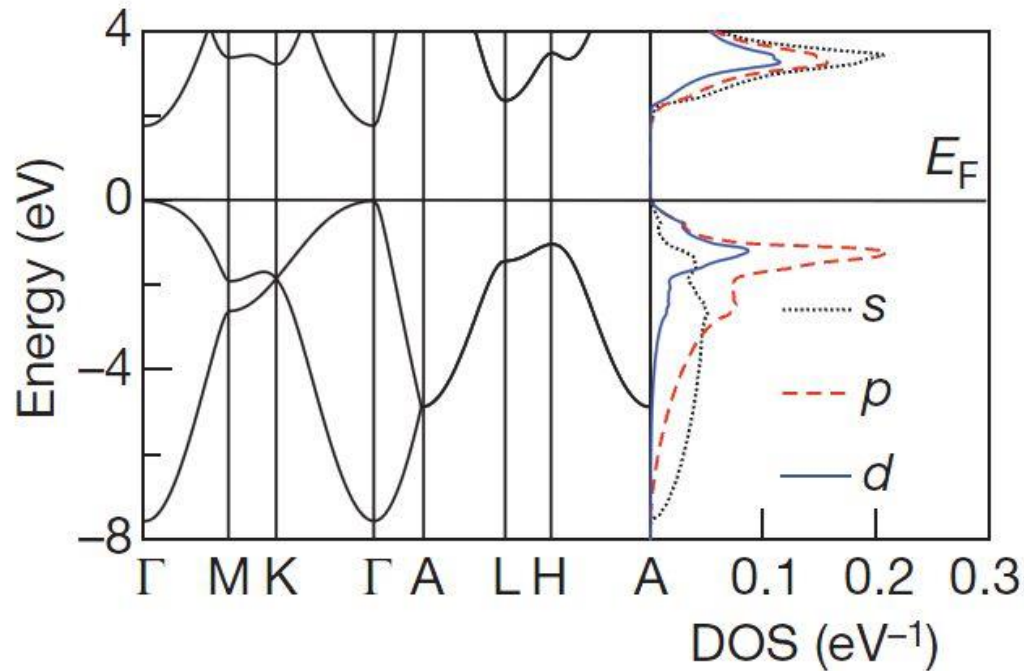
Simulation of Phonon dispersions



The calculated Phonon frequencies (solid lines) and DOS of zinc-blende CuCl at the experimental lattice constants, along with the experimental phonon dispersion data (symbols).

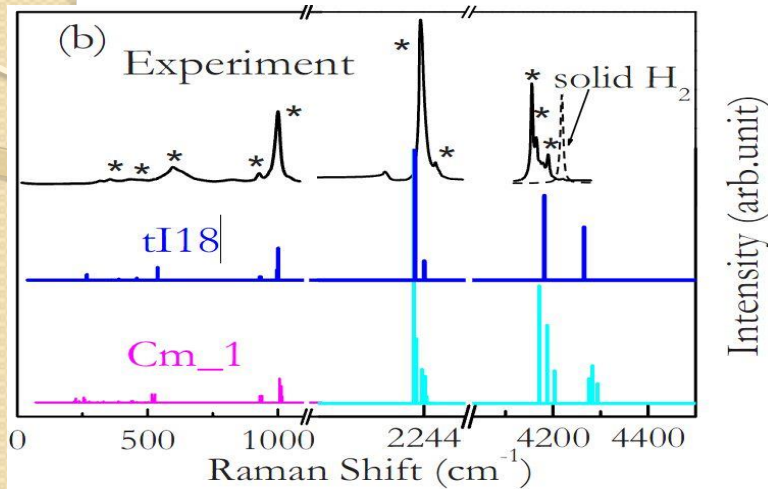
- **Quantum of lattice vibration is called the phonon**
- **Phonon dispersion is a very important criterion for the stabilization of materials.**
- **The calculation of phonon dispersion normally takes several hours to several days.**
- **We can see that the computer simulation can provide precise results.**

Simulation of electronic energy bands



- The band structure of a material determines several characteristics, in particular its electronic and optical properties.
- The band structure calculation is very fast and takes few minutes on high-performance computers.

Simulation of Raman spectroscopy



The simulation of Raman spectroscopy often take several hours on 8 CPUs computer.

- **Raman spectroscopy** (named after Sir [C.V. Raman](#)) is a [spectroscopic](#) technique used to observe vibrational, rotational, and other low-frequency modes in a system.
- Raman spectroscopy is commonly used in chemistry, since vibrational information is specific to the chemical bonds and symmetry of molecules. Therefore, it provides a fingerprint by which the molecule can be identified.
- In solid state physics, spontaneous Raman spectroscopy is used to, among other things, characterize materials, measure temperature, and find the crystallographic orientation of a sample.

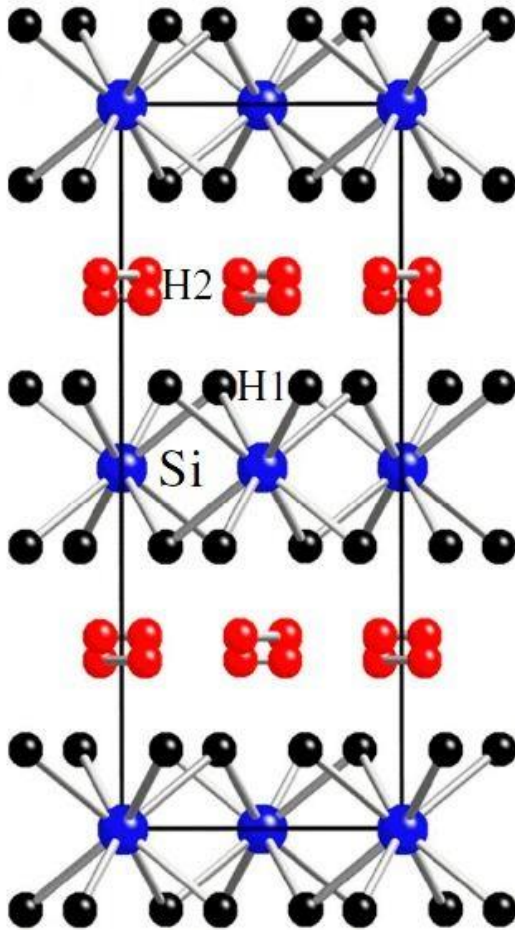
Calculating the superconductivity

- **Superconductivity** :The phenomenon of losing resistivity when sufficiently cooled to a very low temperature.(below a certain critical temperature).
- H.Kammerlingh onnes - 1911 – Pure mercury
- For decades, scientists have been going to great effort to design high-temperature superconducting materials.



- ⦿ The crucial issue in design of high temperature superconductor is to calculate the superconducting critical temperatures.
- ⦿ The calculation of superconducting temperatures is very expensive. It is an almost impossible task about 7 years ago.
- ⦿ It is possible now by high-performance computing.

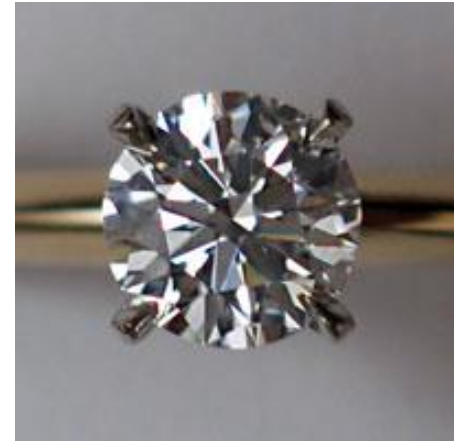
Superconductivity at ~ 100 K in $\text{SiH}_4(\text{H}_2)_2$



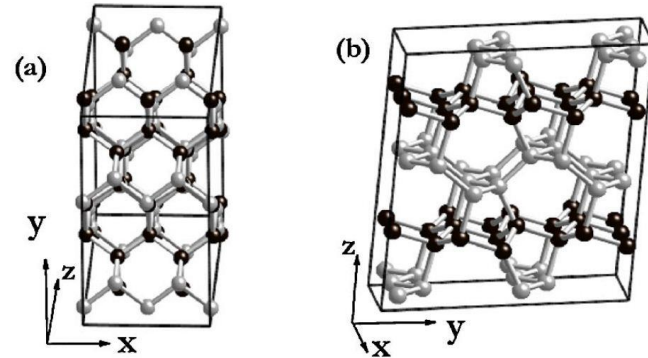
- Owing to the power of high performance computing, one can able to design a novel high-temperature superconductor, $\text{SiH}_4(\text{H}_2)_2$.
- Scientists were used more than 100 CPUs by about one month to calculate the superconducting temperature of $\text{SiH}_4(\text{H}_2)_2$.
- Application of computer simulation yields remarkably high superconducting temperatures of 107 K at 250GPa, among the highest values reported so far for phonon-mediated superconductors.
- Ref: published in PNAS (vol. 107, 15708, September 7, 2010).

Design of superhard materials

- A **superhard material** is a material with a hardness value exceeding 40 gigapascals (**GPa**)
- **Superhard materials are widely used in many applications, from cutting and polishing tools to wear-resistant coatings.**
- **Ten years ago, the hardness of materials can only be measured by experiments.**
- **Now, advances in theory and the high performance computing makes the simulation of the hardness possible.**
- **Therefore, scientists are able to design novel new super hard materials.**



Carbon that cracks diamond

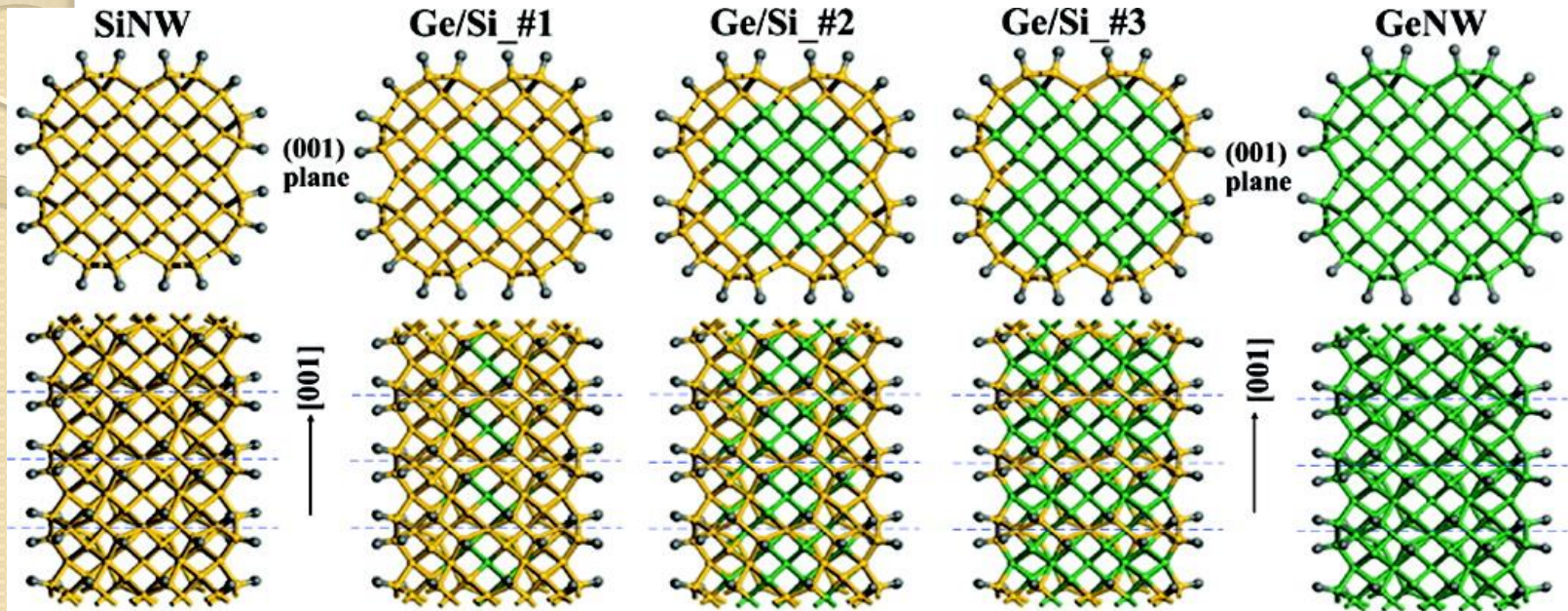


- Scientists have designed a new super hard materials (M-carbon), and simulated the hardness.
- The predicted hardness for M-carbon is 83.1 GPa, which is much higher than that of c-BN (62.4 GPa) and comparable to that of diamond (94.4 GPa).
- *Ref: Published in Physical Review Letter (vol. 102, 175506, 2009), and was highlighted by **Nature News**.*

Design of thermoelectric materials

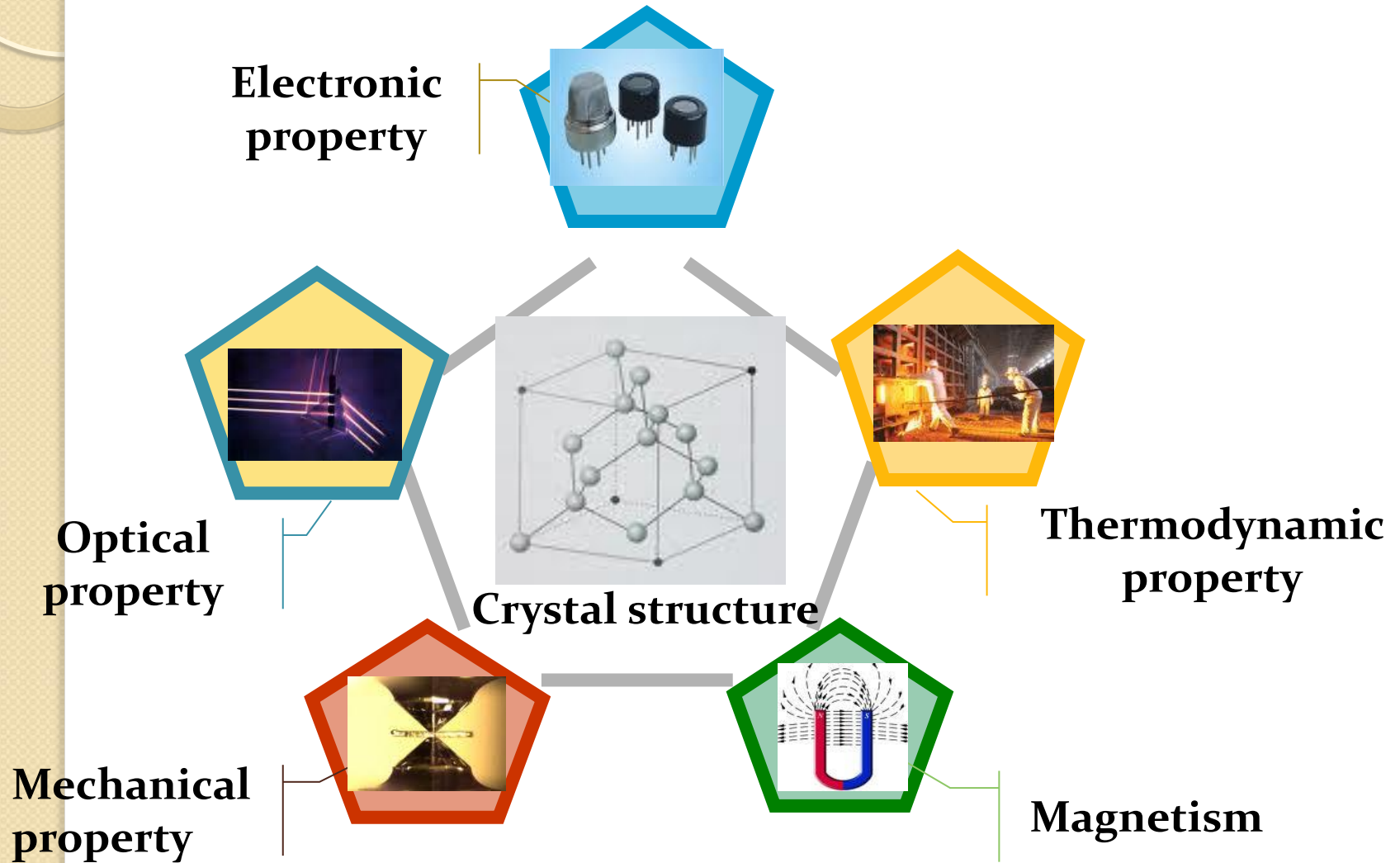
- **Thermoelectric materials are materials which show the thermoelectric effect in a strong and/or convenient form.**
- **Currently there are two primary areas in which thermoelectric devices can lend themselves to increase energy efficiency and/or decrease pollutants: conversion of waste heat into usable energy, and refrigeration.**
- **The efficiency of thermoelectric devices depends on the figure of merit, ZT .**
- **The ZT value can be simulated using high-performance computer.**

Design of novel thermoelectric Ge/Si core-shell nanowires

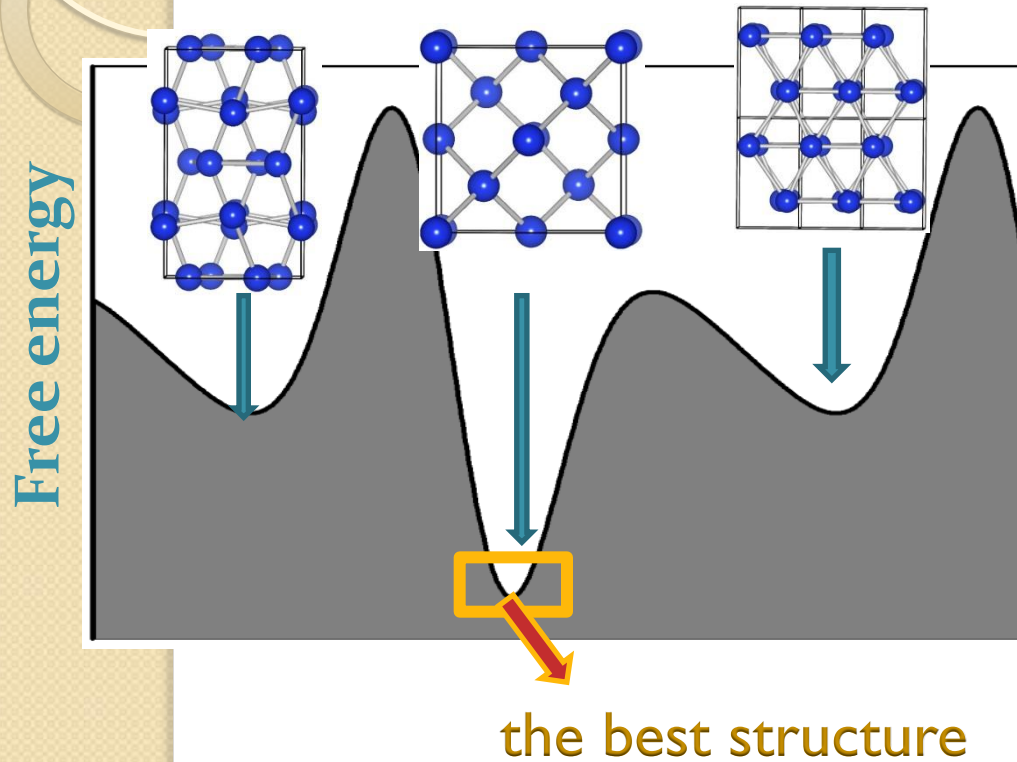


- Scientists calculated the ZT value of Ge/Si core-shell nanowires, and the ZT value is 0.85 at 300K.
- The computing time in simulating ZT value takes about several days on 8 CPUs parallel computer.

Crystal Structure is the basis for understanding materials and their properties



Crystal structure prediction through high performance computing becomes possible

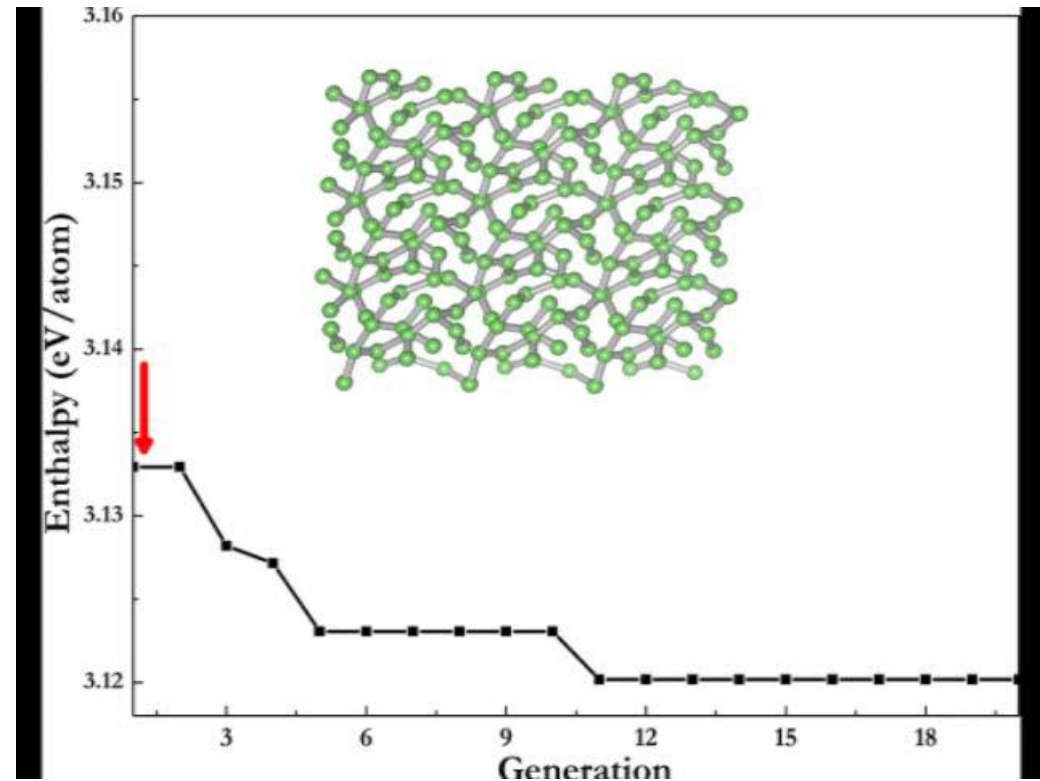


- ◎ The stable crystal structure is the structure with the lowest free energy.
- ◎ So the task is to find the global lowest free energy.

Researchers recently developed a reliable **CALPSO** (crystal structure analysis by particle swarm optimization) code for structure prediction

Structure Evolution of Li under pressure

- Prediction of the crystal structure of Li at 80 GPa.
- Investigators found a new structure that was never to be discovered.



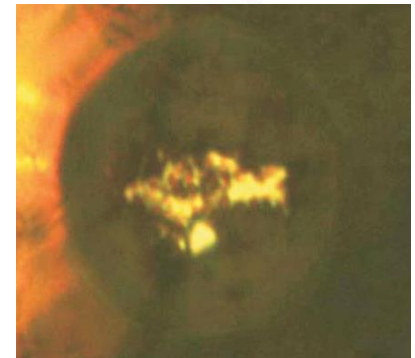
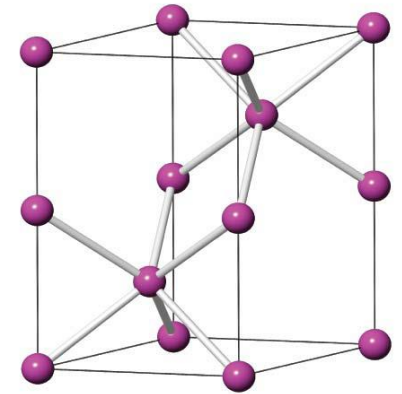
- This calculation takes more than 1 month on parallel computer with 32 CPUs.

Transparent dense sodium



- Sodium is a silvery-white, highly reactive good metal at ambient pressure.

- Researchers have spent several weeks to search new structures of Sodium under high pressures.
- They found that a novel metal-insulator transition in sodium at mega bar pressures against the traditional belief.
- Ref: Published in *Nature* (Vol. 458, 182, 2009).



Conclusion

- **High-performance computing has become the irreplaceable tool in the scientific research on condensed matter physics.**
- **Computer “experiment” can now in some ways be regarded as true “experiment”.**
- **Further development of high performance computing technique could lead new era of condensed matter physics.**



Thank you !!!