



The Abdus Salam
International Centre for Theoretical Physics



2220-7

**15th International Workshop on Computational Physics and Materials
Science: Total Energy and Force Methods**

13 - 15 January 2011

**Crystal Structure Prediction via Particle Swarm Optimization (PSO): Theory and
applications**

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15th Total energy workshop, Trieste, Italy, Jan. 13-15, 2011

**Crystal Structure Prediction via Particle Swarm
Optimization (PSO): Theory and applications**

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2011.1.14

Outline

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Introduction

2

Principles of Particle Swarm Optimization

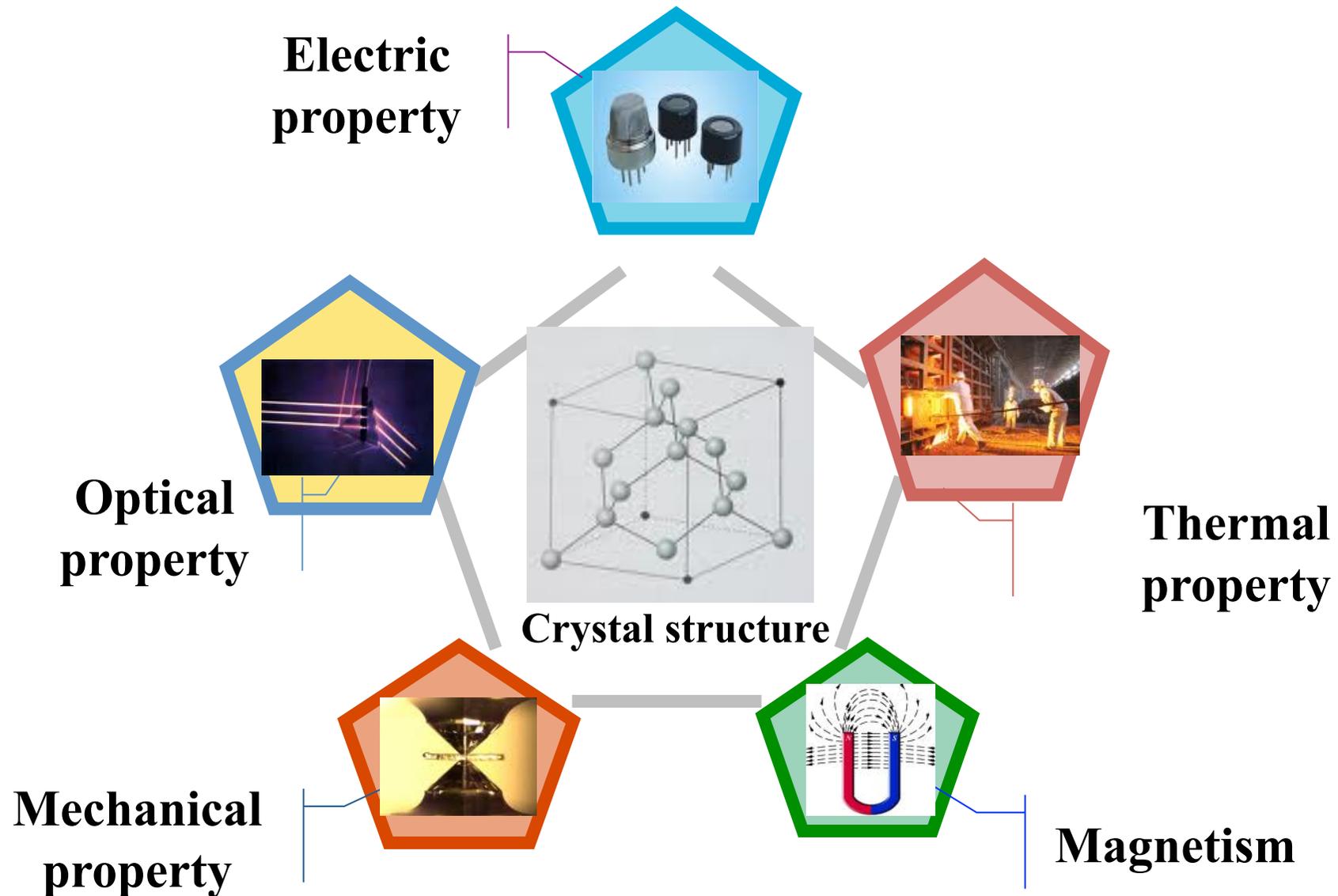
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Benchmark and Applications

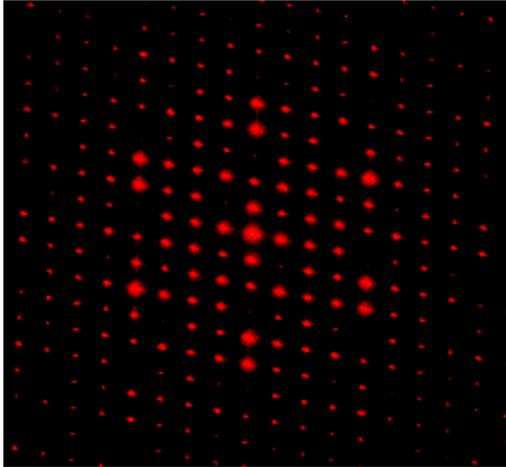
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Conclusions and Perspectives

Structure is the basis for understanding materials and their physical properties



Experimental methods for structural determination



X-ray diffraction



Neutron scattering

Experiments :

- **X-ray diffraction**
- **Neutron scattering**
- **X-ray diffraction and high resolution SEM**

Difficulties :

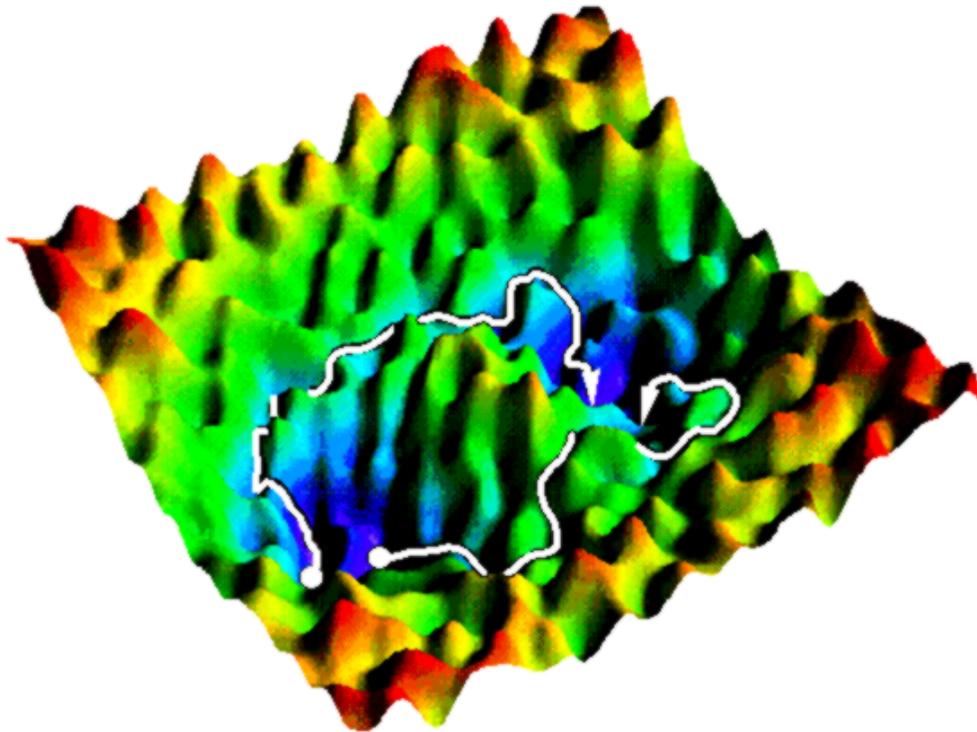
- **Impurity of the sample**
- **Poor diffraction data**
- **Extreme external conditions (e.g., high pressure)**

Crystal structure prediction is essential

What is the challenge of crystal structure prediction?

Finding the GLOBAL stable structure (i.e., energy minimum) on the complex energy landscape with **only given chemical compositions**

Trying all possible structures is **impossible !!!!**



N_{atoms}	Structural Variants
20	10^{25}
30	10^{39}

$$C = \frac{1}{(V/\delta^3)} \frac{(V/\delta^3)!}{[(V/\delta^3) - N]! N!}$$

Earlier Methods and Principles

1. Use of available structure database

- **Data Mining [Christopher, Nat. Mater. 5, 641 (2006)]**
- **Substitutional Method [Mujica, PRB 55, 9659 (1997)]**

2. Random sampling approach

- **C. Pickard and R. Needs [PRL 97, 045504 (2006)]**

“simple” in principle but nontrivial in practice

Earlier Methods and Principles

3. Energy barrier Hopping

- Simulated Annealing [Kirkpatrick, Science 220,671 (1983)]
- Metadynamics [Martonak, PRL 90, 75503 (2003)]
- Basin Hopping [Wales, JPCA 101, 5111 (1997)]
- Minima Hopping [Goedecker, JCP 120,9911 (2004)]

Conquering the energy barrier

4. Genetic algorithm (GA)

- Bush, JMC 5, 1269 (1995) ; Woodley, PCCP 1, 2535 (1999)
- Deaven , PRL 75, 288 (1995)
- USPEX [Oganov, JCP 124, 244704 (2006)]
- GSGO [Zunger , PRB 75, 104113, 2007]

Operation: cross over and mutation

Advantage: self-improving via evolution

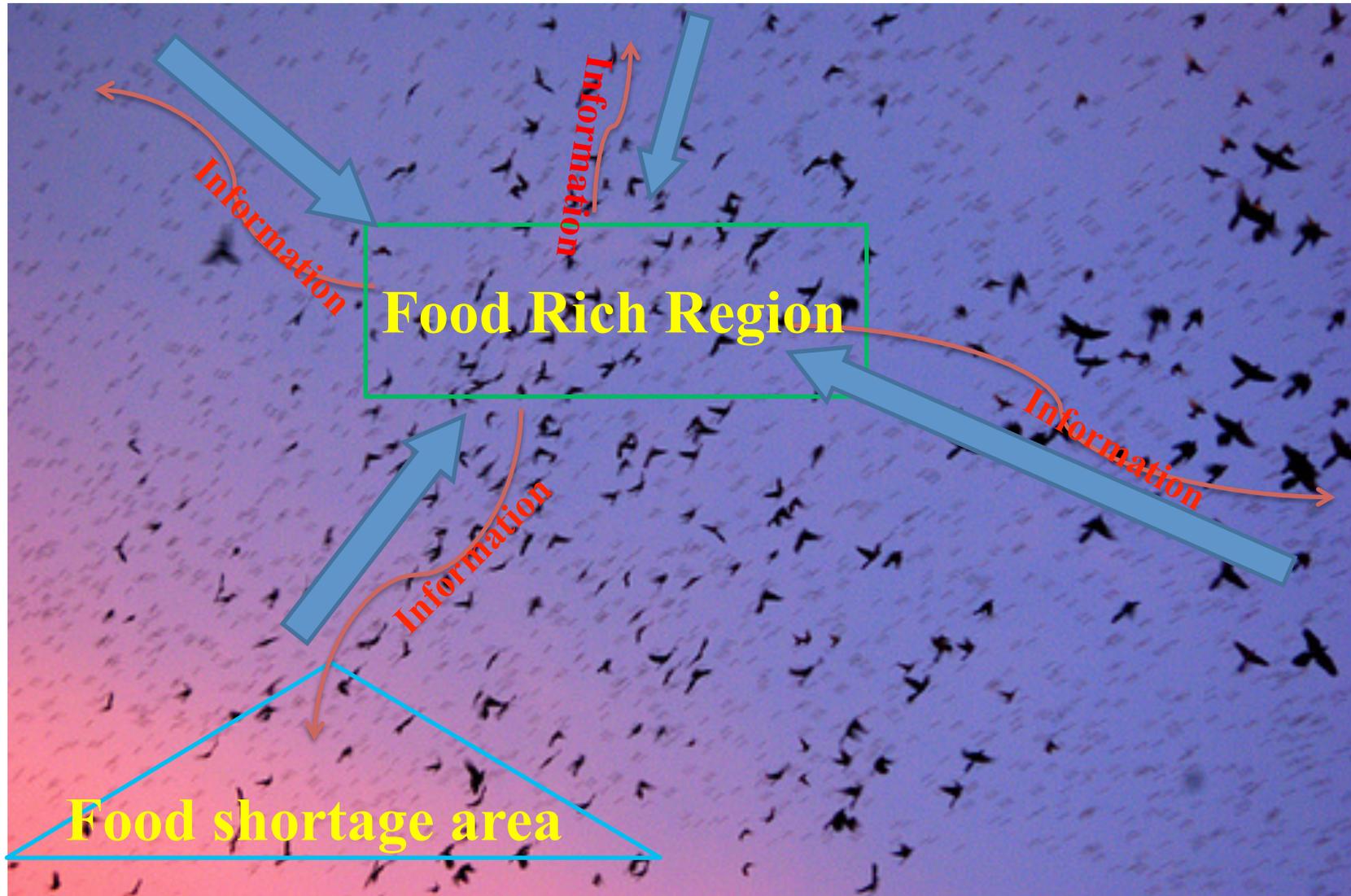
Particle Swarm Optimization (PSO)

Kennedy and Eberhart 1995

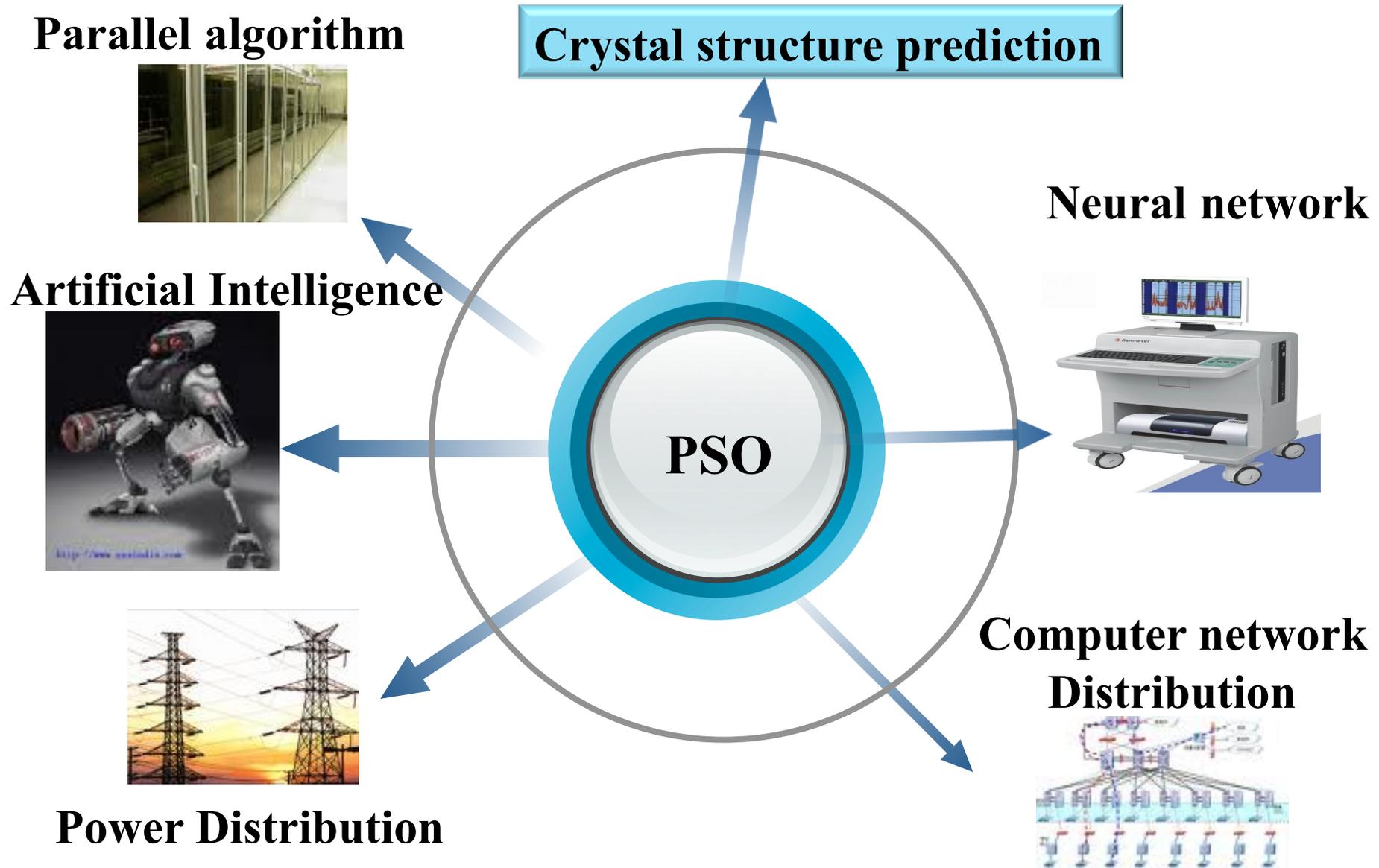


- Swarm search
- Information exchanges between Individual particles
- Self-improving evolution
- Swarm Intelligence
- Particles evolve by tracing with the optimal Particle

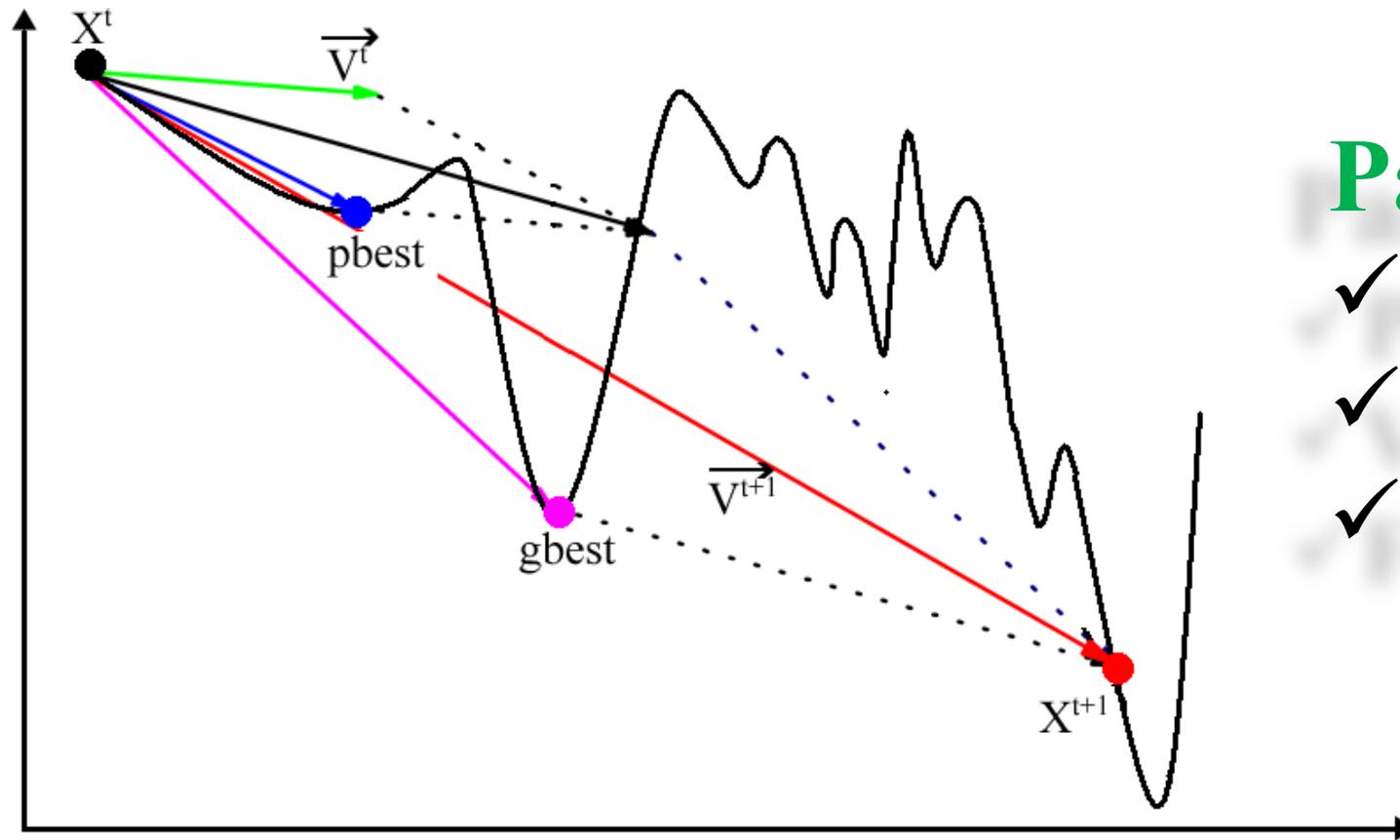
Principle of PSO



Application of PSO on crystal structure prediction



PSO Principle on structural prediction



Particle

✓ **Position**

✓ **Velocity**

✓ **Fitness**

$$x_{i,j}^{t+1} = x_{i,j}^t + v_{i,j}^{t+1}$$

$$v_{i,j}^{t+1} = \omega v_{i,j}^t + c_1 r_1 (pbest_{i,j}^t - x_{i,j}^t) + c_2 r_2 (gbest_{i,j}^t - x_{i,j}^t)$$

CALYPSO code

Crystal structure AnaLYsis by Particle Swarm Optimization

CALYPSO

- **The name of the Nereids (sea nymphs) in Greek mythology**
- **A genre of Trinidadian folk music**

Input parameters: **chemical compositions and external conditions (e.g. high pressure)**

Wang, Lv, Zhu, and Ma, Phys. Rev. B 82, 094116 (2010)

China copyright protection via No.**2010SR028200**

Features of CALYPSO

1. Randomly generated structures (symmetrical constraint)

Reduction of the search space

Increase of structural diversity to avoid trapping into local minimum

2. Locally Structural Optimization

Reduction of the noise of the energy landscape

3. Geometrical Structure Parameter (Similar function)

Elimination of duplicated structure and determination of non-fly area to improve search efficiency

4. Particle Swarm Optimization (Swarm Intelligence and self-improving)

Swarm Intelligence through information exchanges

Control of particle speed and direction by optimal particle to accelerate convergence

Excluding unfavorable energy landscape through self-improving to reduce the search space

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Benchmark of CALYPSO

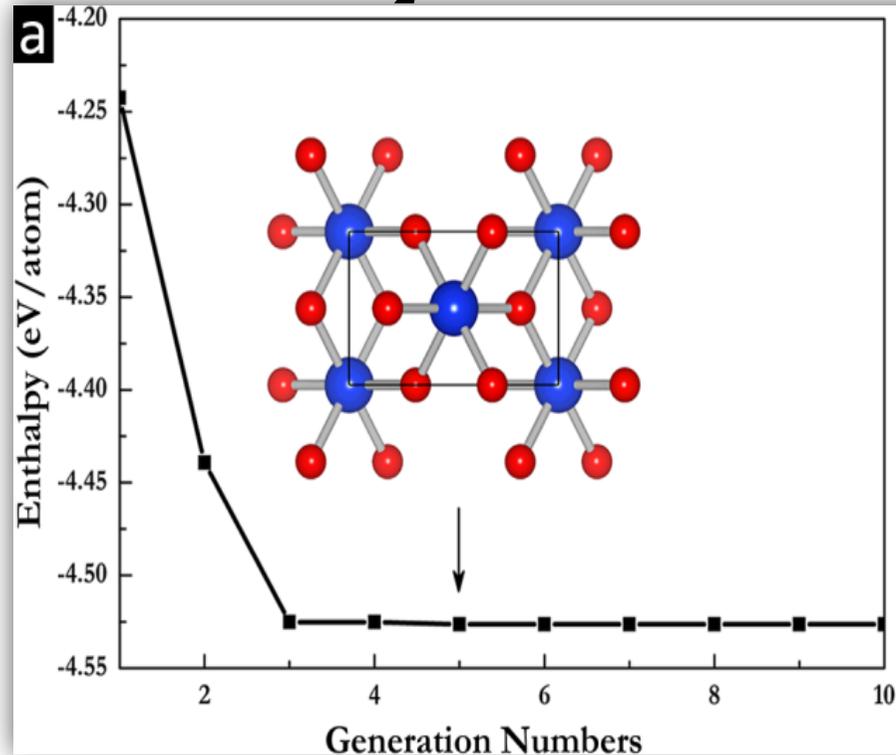
System	Pressure (GPa)	Structure	Generation	Population size
Li	0	Bcc	1	30
	0	9R	3	30
	10	Fcc	1	20
	40	hR1	4	30
	70	cI16	7	30
C	0	Graphite	30	30
	0	Diamond	6	30
Si	2	Bc8	6	30
	10	cd	1	20
	10	sh	2	20
	10	β - Sn	3	20
	10	<i>Imma</i>	4	20
	40	<i>Cmca</i>	2	20
	40	Hcp	4	20
	80	Fcc	1	20
Mg	0	Hcp	6	30
	100	Bcc	4	30

Benchmark of CALYPSO

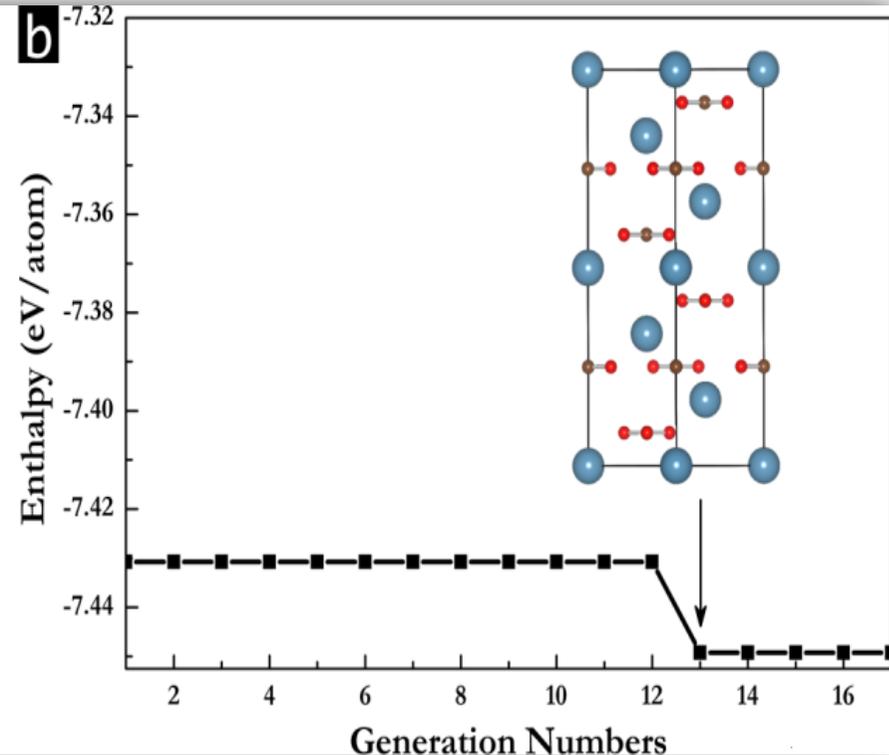
System	Pressure (GPa)	Structure	Generation	Population size
SiO ₂	0	α -quartz	5	20
	20	Stishovite	1	20
	70	CaCl ₂ -type	5	30
	100	α -PbO ₂ -type	4	20
	500	Pyrite-type	15	20
SiC	0	Zinc blende	6	30
	0	Moissanite	3	30
	150	Rock salt	2	30
ZnO	12	Rock salt	2	30
TiH ₂	0	<i>I4/mmm</i>	2	20
	0	Fm-3m	3	20
MoB ₂	0	R-3m	1	30
TiB ₂	0	AlB ₂ -type	1	30
MgSiO ₃	120	<i>Cmcm</i>	5	20
CaCO ₃	0	Calcite	13	30

Benchmark of CALYPSO

CaCl₂ structure



Calcite structure



SiO₂ at 70GPa

CaCO₃ at 0GPa

Wang, Lv, Zhu, and Ma, Phys. Rev. B 82, 094116 (2010)

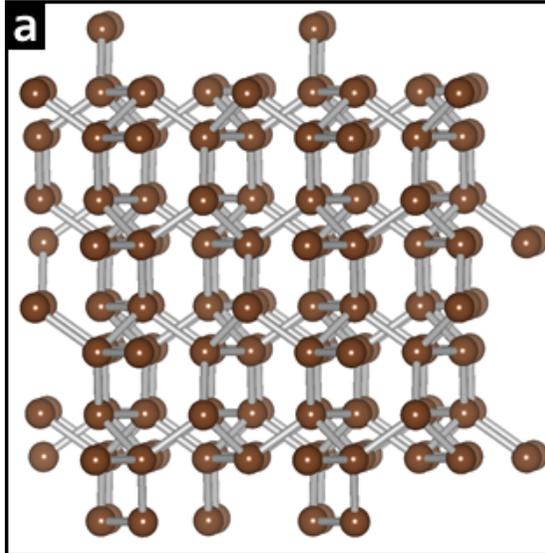
Comparison with GA

Systems	Algorithm	Pressure (GPa)	Structures	Generations	N_{pop}	N_{opt}
Si	PSO	0	Diamond	8/5	16	128/5
	GA ^a	0	Diamond	15	16	60
SiC	PSO	0	Zinc blende	8/5	12	96/5
	GA ^a	0	Zinc blende	5	12	20
GaAs	PSO	0	Zinc blende	16/5	12	192/5
	GA ^a	0	Zinc blende	19	12	70

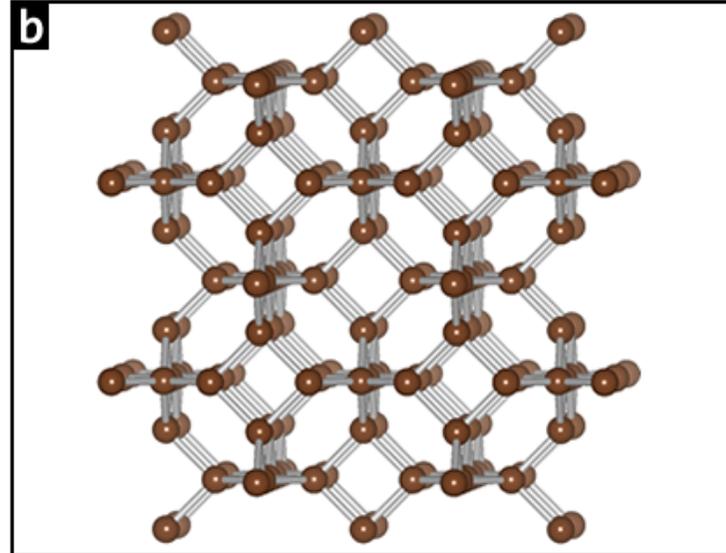
**GA data taken from
Trimarchi and Zunger, PRB 75, 104113 (2007)**

Carbon polymorphs by CALYPSO

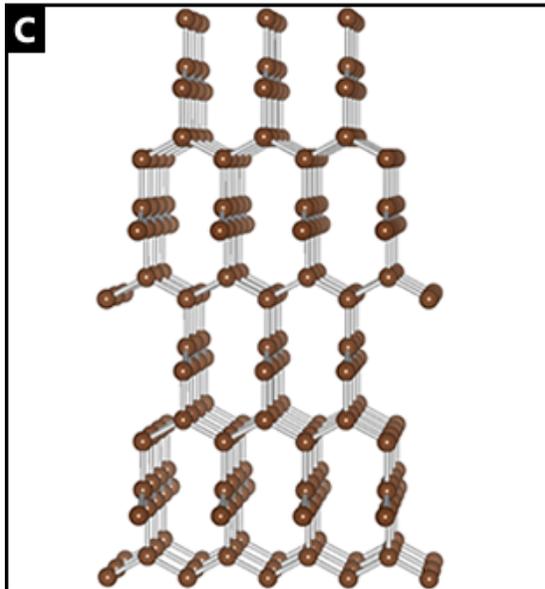
BC_8



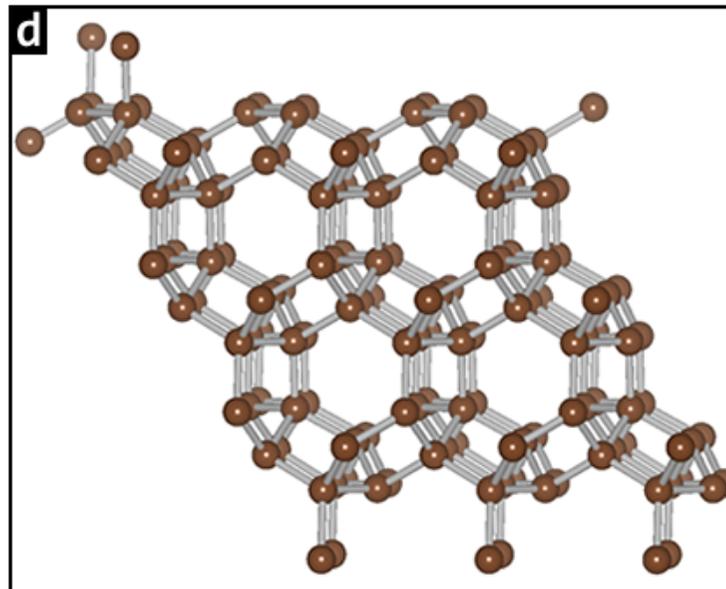
C_6



β -Sn



$P6_522$



Metastable phases of Carbon



Metal-insulator transitions in Lithium and Sodium under pressure

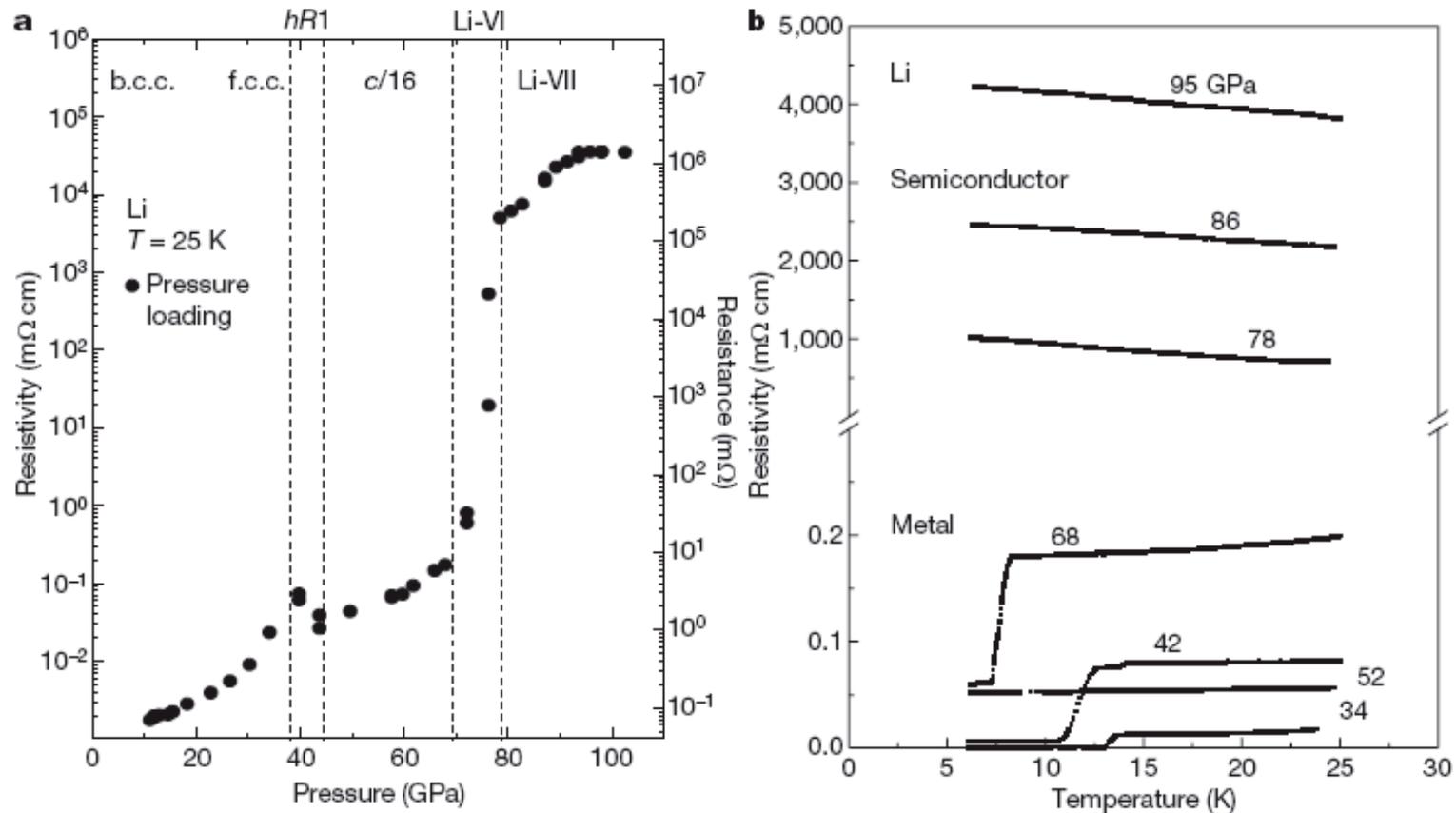
**Yanming Ma, et al., “Transparent dense sodium”,
Nature 458, 182 (2009)**



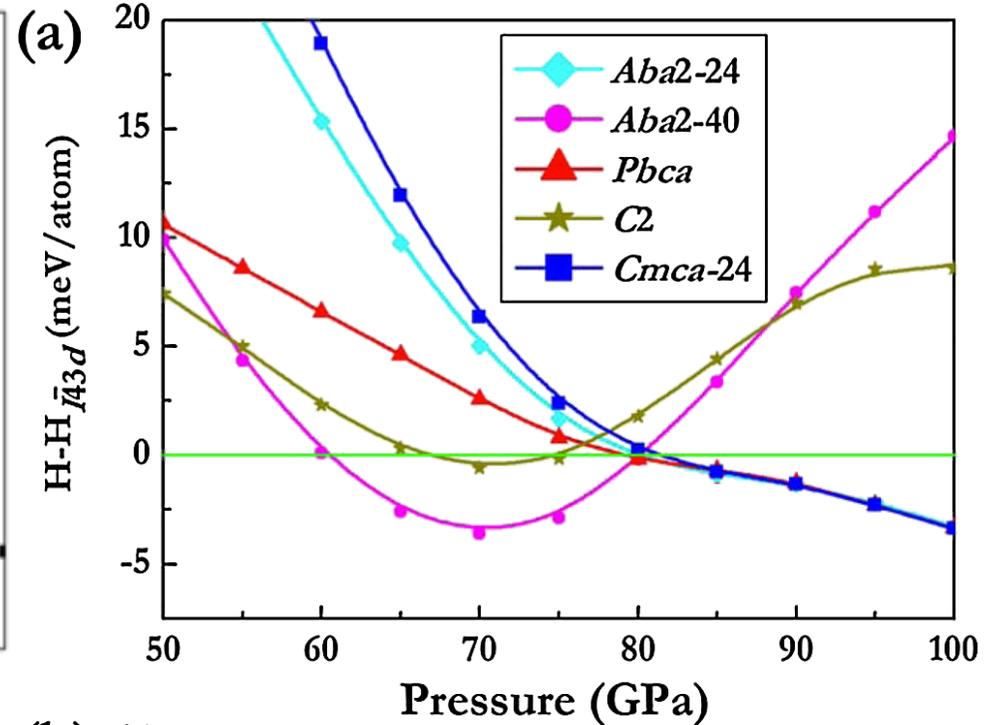
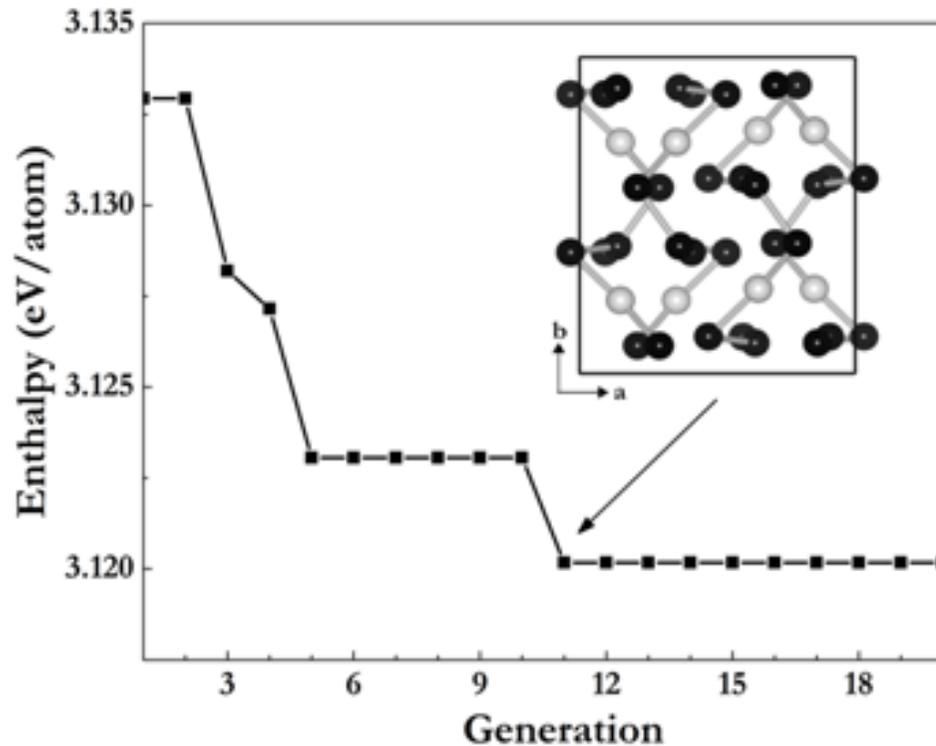
High pressure insulating structures of Li

Direct observation of a pressure-induced metal-to-semiconductor transition in lithium

Takahiro Matsuoka¹ & Katsuya Shimizu¹

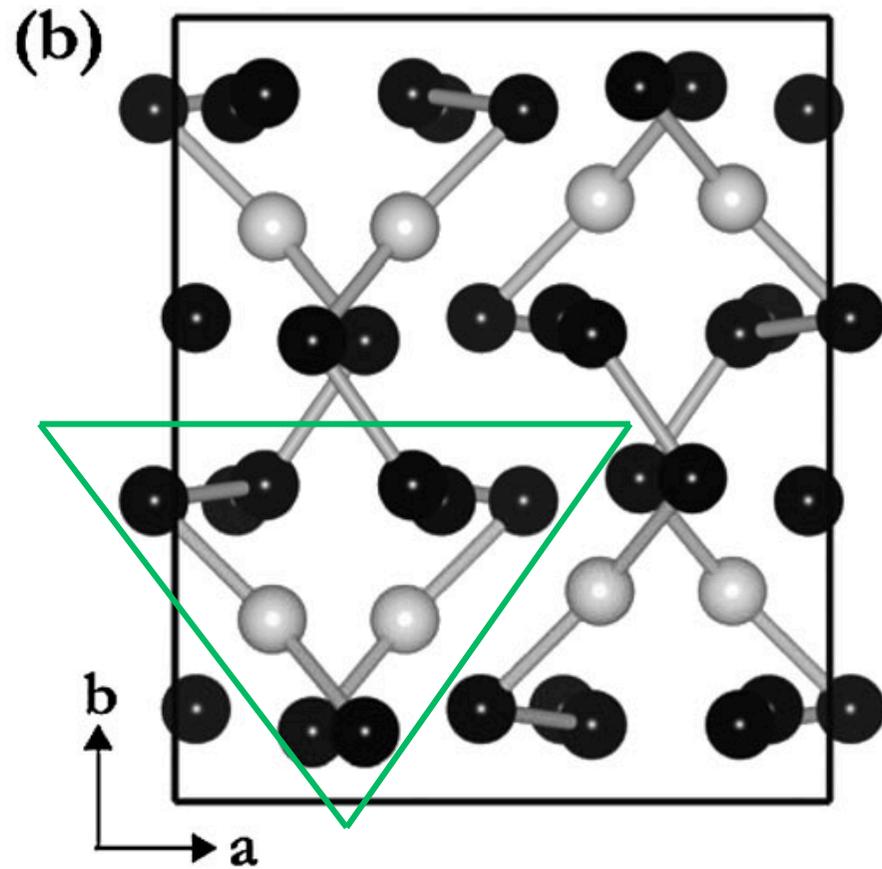
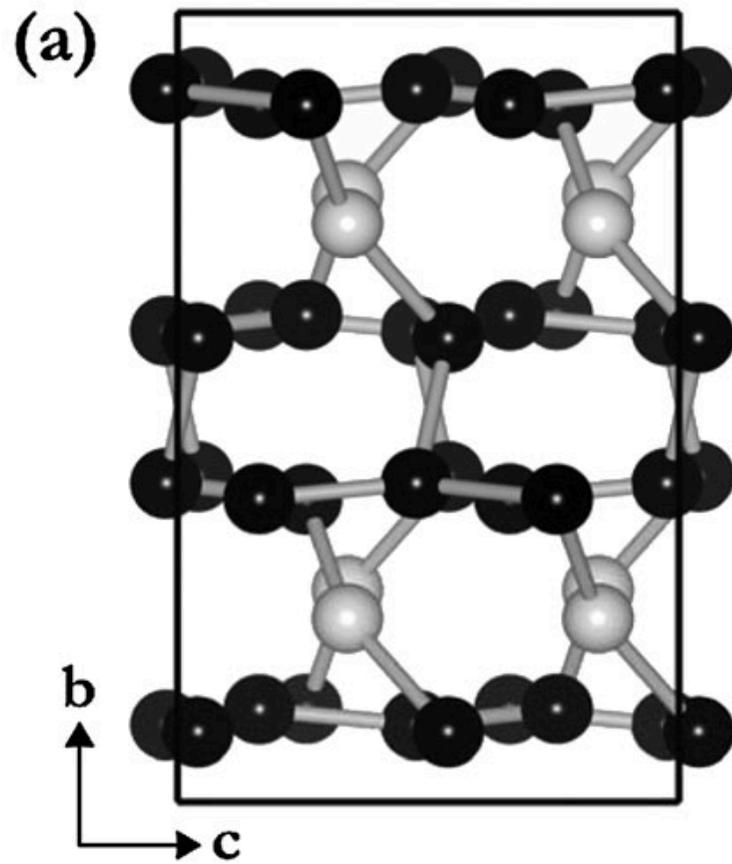


Prediction of the most favorable insulating structure of Li

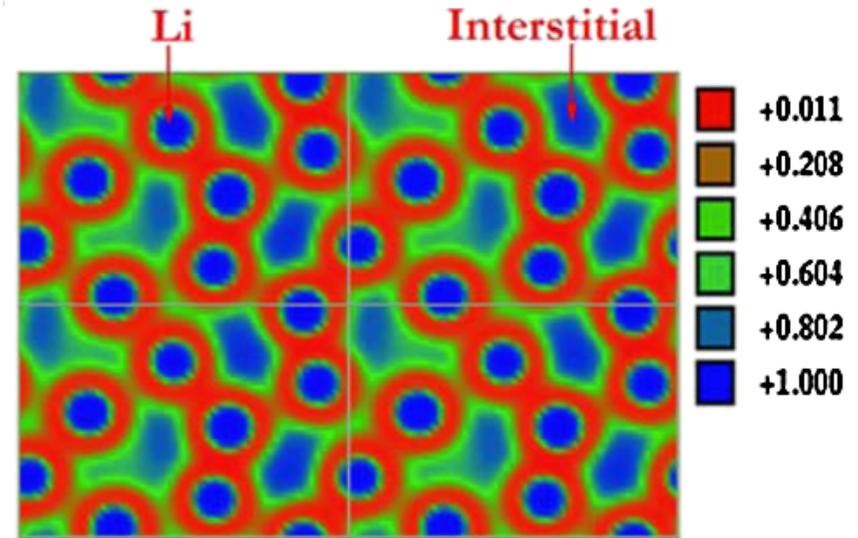
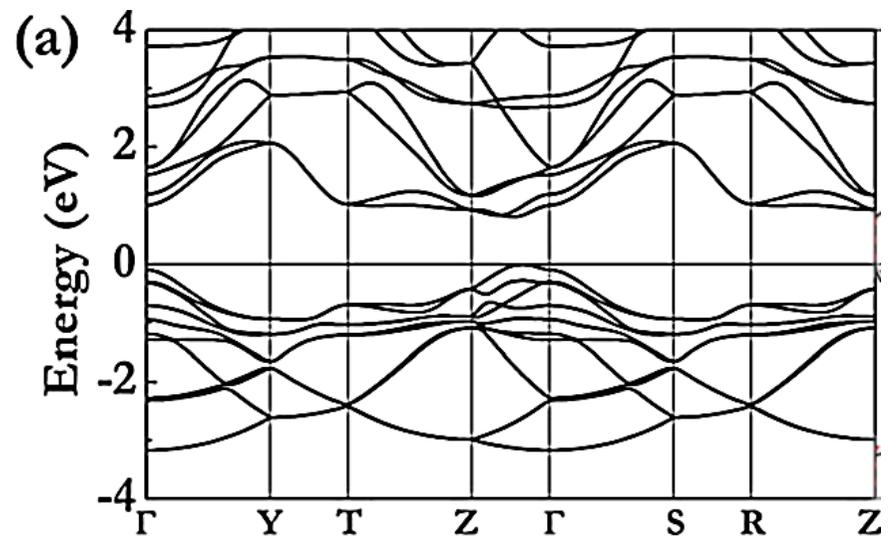


Li at 80 GPa (Aba2-40)

Lv, Wang, Zhu, and Ma, PRL 106,015503 (2011)



Li at 80 GPa (orthor.)



Experimental confirmation?

Cold melting and solid structures of dense lithium,
Guillaume1, *et al*, Nature physics, DOI: 10.1038/
NPHYS1864, (2011)

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Conclusions

PSO on crystal structure prediction

1. Wide range of applications

Metals, semiconductors, insulators and ionic crystals, etc.

2. Fast convergence

Number of local optimization < 300

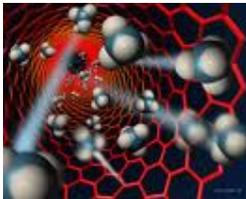
3. High success rate

The success rate of prediction on elemental, binary and ternary compounds is nearly ~100%

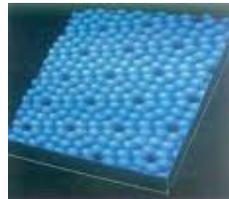
4. Capable on Prediction of meta-stable structures

Perspectives of CALYPSO code

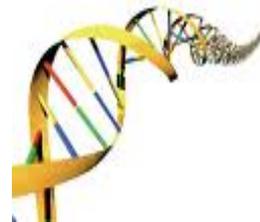
◆ Nano-materials, surface, cluster and bio-materials



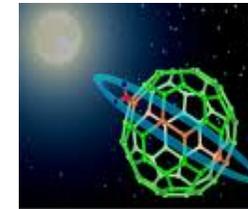
Nano-structure



Surface



Biomaterials



Cluster

◆ Design of novel functional materials

(1) Superconductors (2) Superhard Materials (3) Thermoelectric materials

Welcome to use CALYPSO package

Webpage: <http://nlshmlab.jlu.edu.cn/~calypso.html>

Please send to YM (mym@jlu.edu.cn) for request



Thanks ! ! !

