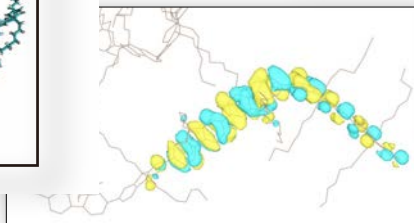
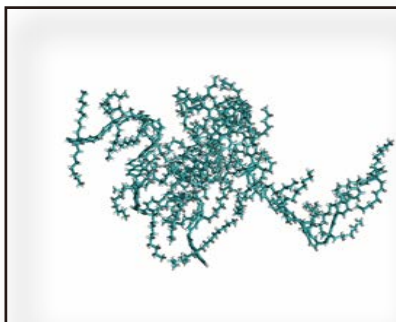


# Novel linear algebraic theory and one-hundred-million-atom quantum material simulations on the K computer

T. Hoshi(星健夫)<sup>1</sup>, T. Sogabe(曾我部知広)<sup>2</sup>, T. Miyata(宮田考史)<sup>3</sup>, S.-L. Zhang(張紹良)<sup>3</sup>

1. Tottori University, Japan, 2. Aichi Prefecture University, Japan;

3. Nagoya University, Japan



$$Hy = \lambda Sy$$

$$(zS - H)x = b$$



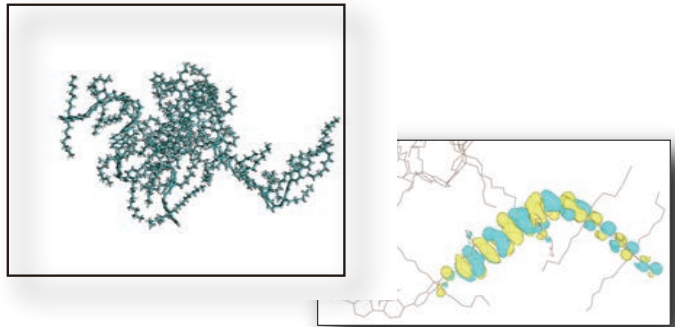
Fund : JST-CREST 'Development of System Software Technologies  
for Post-Peta Scale High Performance Computing'  
and so on.



# Application-Algorithm-Architecture co-design

→ Inter-disciplinary studies between physics, mathematics and HPC

Application : quantum material simulationn



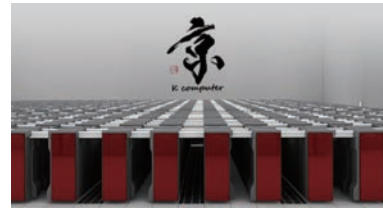
..

Algorithm : numerical linear algebra

$$Hy = \lambda Sy$$

$$(zS - H)x = b$$

Architecture : from supercomputers to personal computers



# Application-Algorithm-Architecture co-design

→ Inter-disciplinary studies between physics, mathematics and HPC

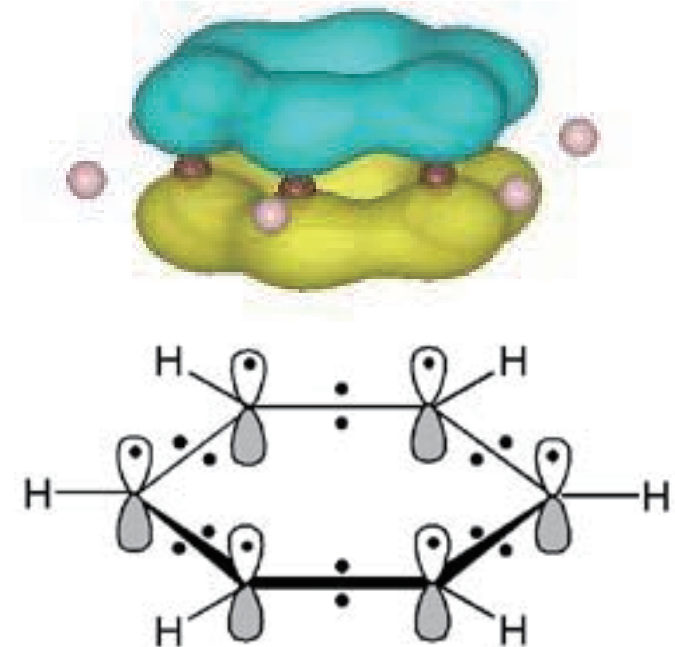
Tutorial : What is electronic state calculation ?

- (a) quantum-mechanical 'wave' theory for electrons in materials
- (b) basics of quantum material simulations
- effective Schrödinger equation
- generalized Hermitian eigen-value problem (as a typical numerical problem)

$$H\mathbf{y} = \lambda S\mathbf{y} \quad (S \approx I)$$

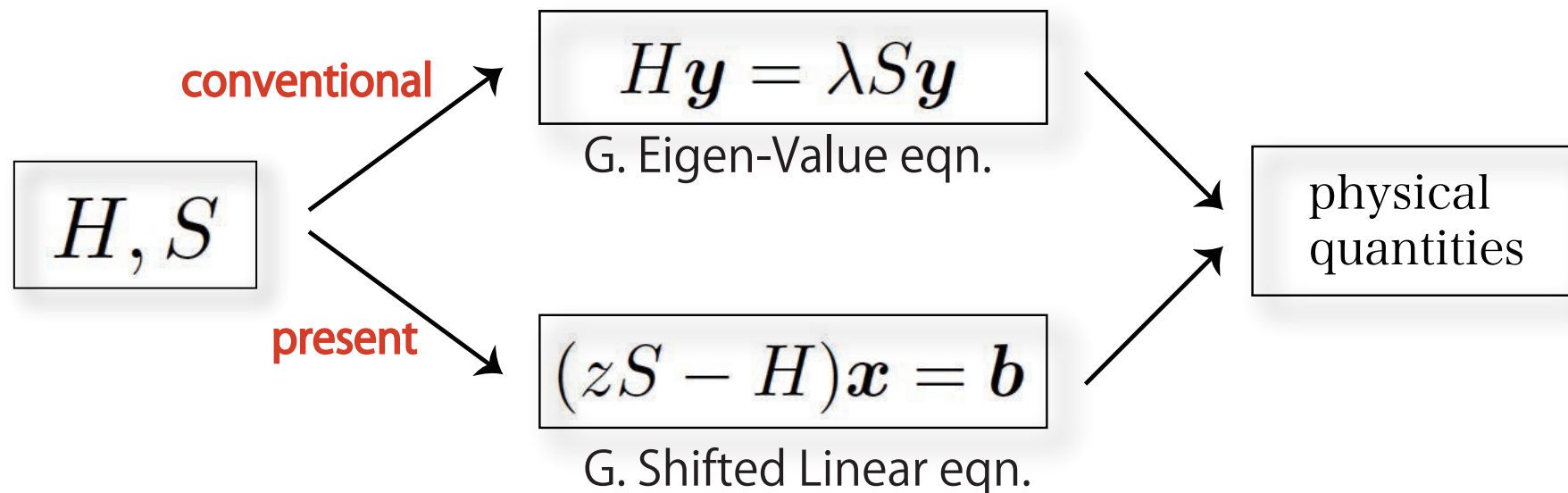
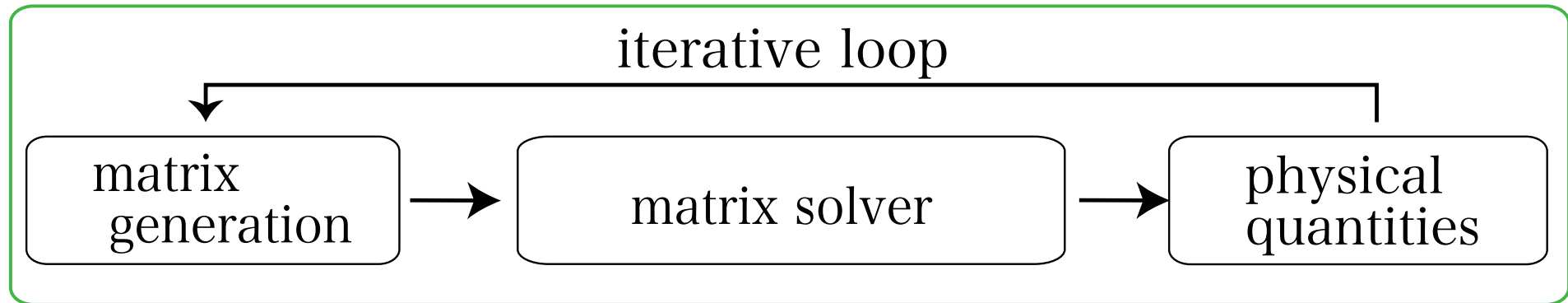
$\lambda$  : energy for each electron ('eigen energy')  
 $\mathbf{y}$  : shape of electronic 'wave' ('wavefunction')(\*)

(\*) An electronic 'wave' (wave function) of Benzene ( $C_6H_6$ )



# Application-Algorithm-Architecture co-design

- Inter-disciplinary studies between physics, mathematics and HPC
- Construct an optimal workflow for each target physical quantity



# Linear algebra : Krylov subspace solver

... is the general name of iterative solvers

with successive matrix-vector multiplications

: Ex. conjugate-gradient, Lanczos, Arnoldi algorithms

The solution is given on the sub(linear)space of

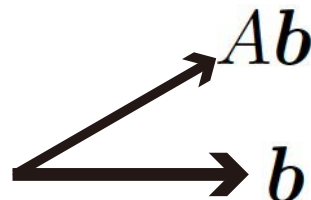
$$K_n(A; \mathbf{b}) \equiv \text{span} \{ \mathbf{b}, A\mathbf{b}, A^2\mathbf{b}, \dots, A^{n-1}\mathbf{b} \}$$

$n$  : subspace dimension (iteration number)

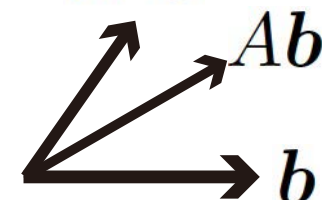
$n=1$



$n=2$



$n=3$   $A^2\mathbf{b}$



# Novel linear algebraic algorithms

- [1] Teng et al., PRB 83, 165103 (2011); [2] Hoshi et al, JPCM 24, 165502 (2012).  
[3] Sogabe JCP 231, 5669 (2012); [4] Yamashita et al., Trans. JSIAM 21, 241 (2011).

→ Iterative (Krylov subspace) solvers for generalized shifted linear equation

$$\underbrace{(H - zS)}_{\text{non-hermitian}} x = b$$

Mathematical principles	$S \neq I$	$S = I^*$
Gerlerkin Principle	gLanczos, gArnoldi, mArnodi, Arnoldi (M;W;G)	subs. diag.
Collinear Residual	gsCOCG, gsQMR	sCOCG, sQMR

\*Takayama *et al.*, JPSJ73, 1519 (2004); Takayama et al. PRB 73, 165108(2006); Sogabe et al. ETNA31, 126 (2008)

## Wide applicability of algorithms

→ Krylov-subspace algorithms for (generalized) shifted linear equation appear among different physics areas

Ex. Papers with the **collinear residual theorem**

(1) **A. Frommer, Computing 70, 87 (2003)** [ Original paper of the theorem]

→ **QCD**

(2) R. Takayama, T. Hoshi, T. Sogabe, S.-L. Zhang, and T. Fujiwara, PRB 73, 165108 (2006).

→ **large-scale electronic structure calculation** [present work]

(3) S. Yamamoto, T. Fujiwara, and Y. Hatsugai, PRB 76, 165114 (2007);

S. Yamamoto, T. Sogabe, T. Hoshi, S.-L. Zhang and T. Fujiwara, JPSJ 77,114713 (2008)

→ **many-body electron** [full-CI type, multi-orbital extended Hubbard model, LaSrNiO]

(4) T. Mizusaki, K Kaneko, M. Honma, T. Sakurai, PRC 82, 024310 (2010)

→ **Shell-model calculation**

(5) F. Giustino, M. L. Cohen, and S. G. Louie, PRB 81, 115105 (2010)

→ **GW (excited electron) calculation**

# Methods used in the data hereafter

(1) One of our novel linear-algebraic solvers

→ multiple Arnoldi algorithm(\*) for generalized shifted linear eq.

$$(H - zS)\mathbf{x} = \mathbf{b} \quad (S \approx I)$$

→ the use of multiple Krylov subspaces of

$$\mathcal{L} \equiv K_p(H; \mathbf{b}) \oplus K_q(H; S^{-1}\mathbf{b})$$

where  $K_n(A; \mathbf{b}) \equiv \text{span} \{ \mathbf{b}, A\mathbf{b}, A^2\mathbf{b}, \dots, A^{n-1}\mathbf{b} \}$

(\*)T. Hoshi, S. Yamamoto, T. Fujiwara, T. Sogabe, S.-L. Zhang,  
J. Phys.: Condens. Matter 24, 165502 (2012)

(2) Other details

- Applicable both to metals and insulators
- Modelled (TB-type) systems, based on ab initio calculation
- A DFT-derived charge-self-consistent formulation (optional)



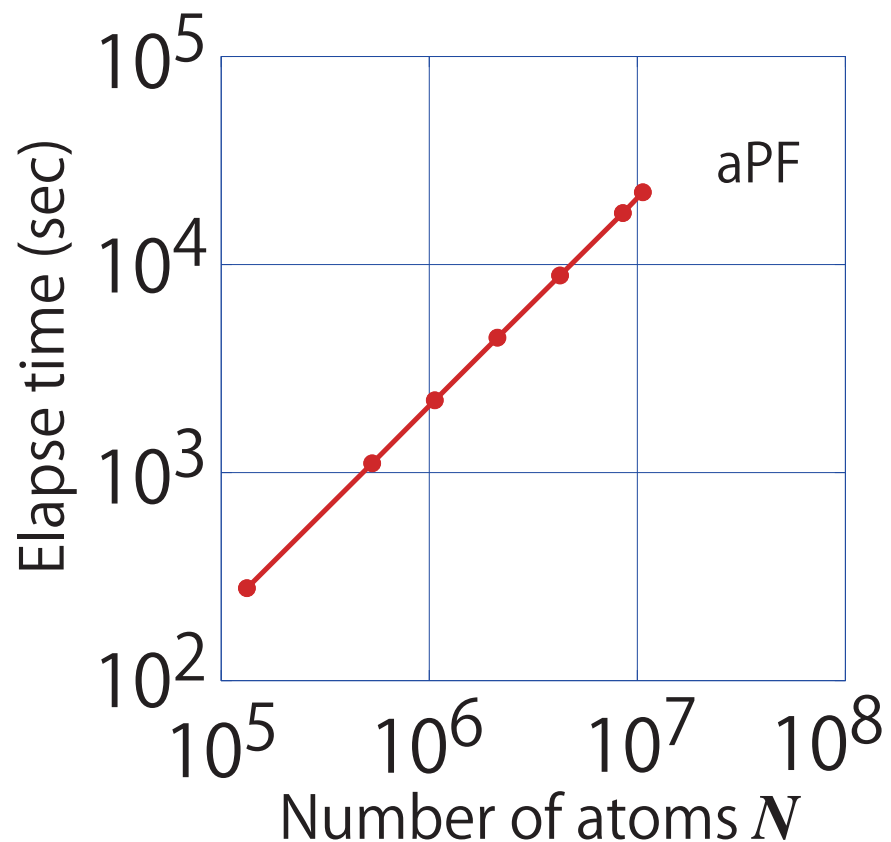
# ELSES, our electronic-structure calculation code

Hoshi et al., JPSJ 82, 023710 (2013); Hoshi et al., Preprint (<http://arxiv.org/abs/1307.3218>)

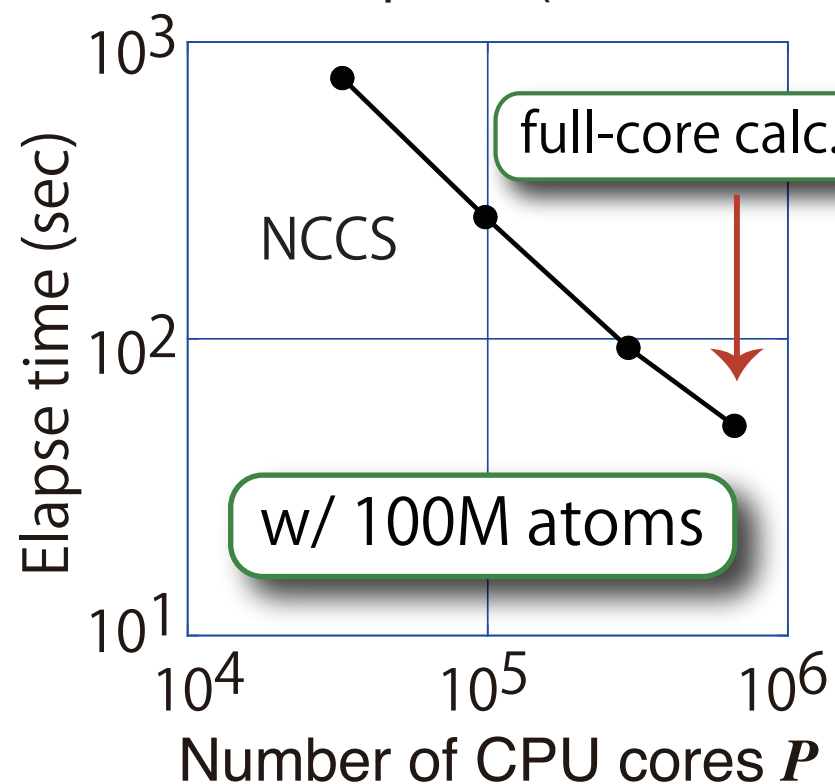
Benchmark with upto 100M atoms ( $\rightleftharpoons$  Si :  $(126\text{nm})^3$  region)

aPF : amorphous-like conjugated polymer, poly-(9,9 dioctyl-fluorene),  
NCCS: sp<sup>2</sup>-sp<sup>3</sup> nano composite carbon solid

(a) Order- $N$  scaling



(b) Parallel efficiency (strong scaling) on the K computer ( $\sim$  all nodes)

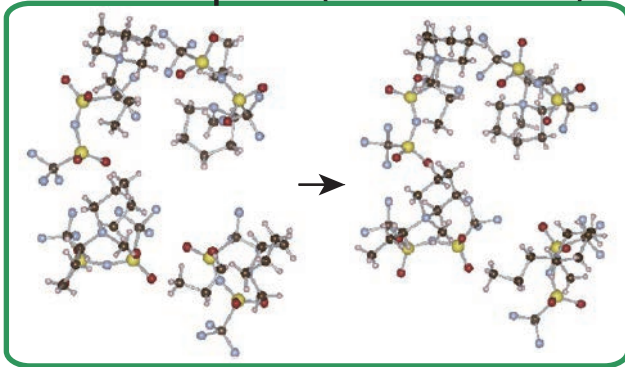


# Examples of nano-material studies with 'ELSES'

## Motivations

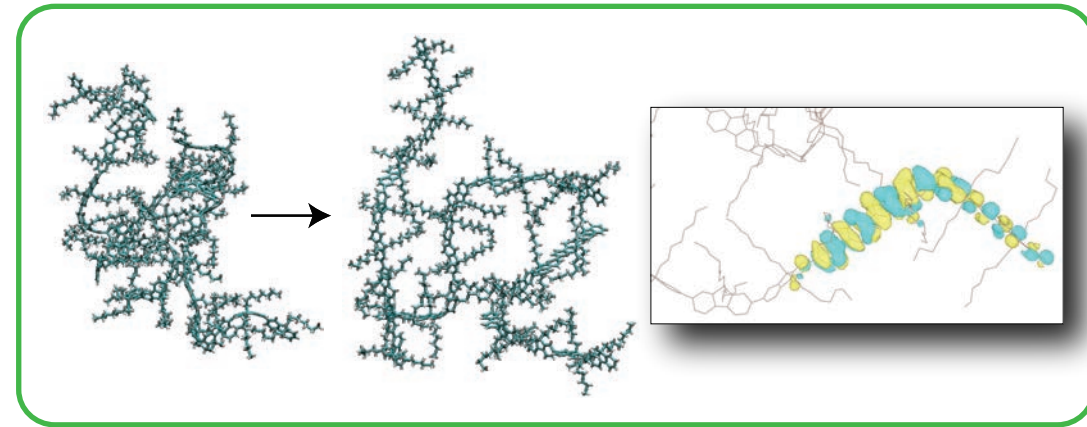
- (i) industrial application
- (ii) new material (from Japan)
- (iii) standard material

## Ionic liquid (PP13-TFSI)

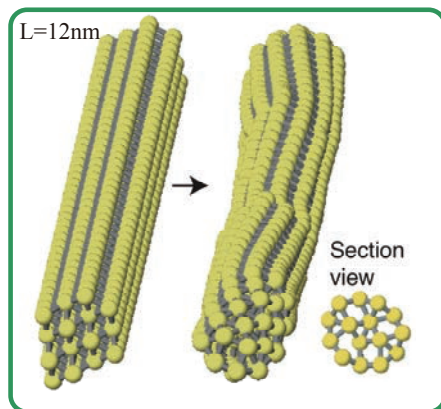


$\text{Li}^+$  diffusion  
in solids  
(Nishino et al.)

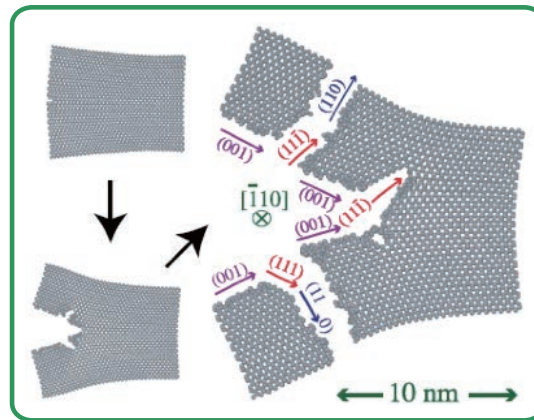
## Amorphous-like conjugated polymer (poly-(9,9 dioctyl fluorene))



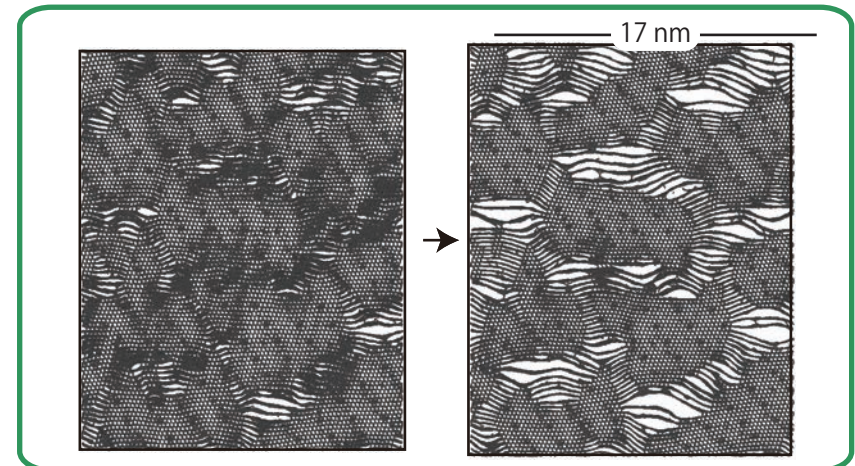
## helical gold nanowire



## silicon brittle fracture



## sp<sup>2</sup>-sp<sup>3</sup> nano-composite carbon solid ( for nano-polycrystalline diamond )

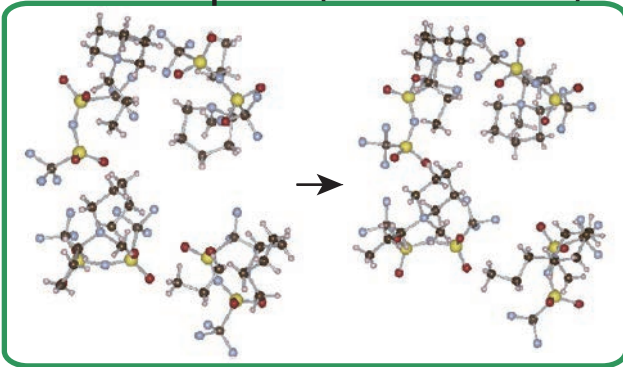


# Examples of nano-material studies with 'ELSES'

## Motivations

- (i) industrial application
- (ii) new material (from Japan)
- (iii) standard material

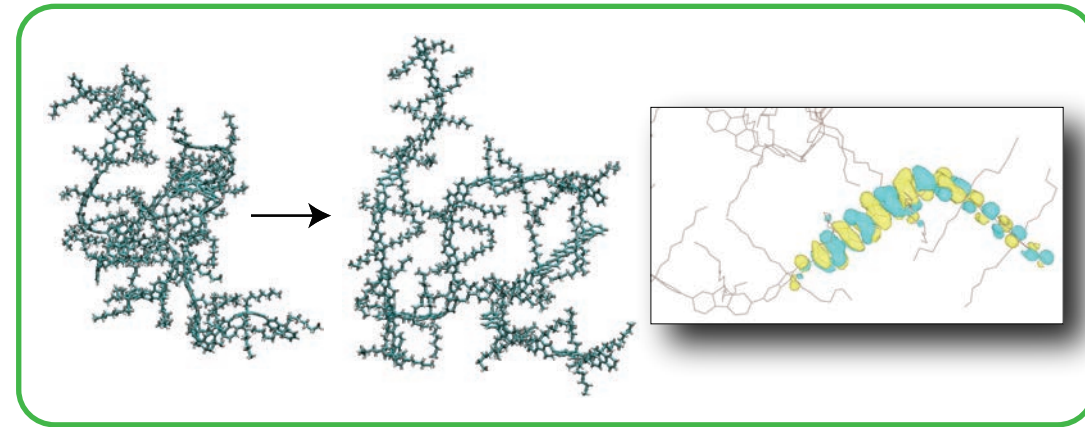
## Ionic liquid (PP13-TFSI)



Li<sup>+</sup> diffusion  
in solids

Recent paper :  
S. Nishino (U Tokyo)  
T. Fujiwara (U Tokyo),  
H. Yamasaki (Toyota),  
S. Yamamoto (Tokyo U. Tech.),  
T. Hoshi (Tottori U),  
Solid State Ionics 225,  
22-25 (2012).

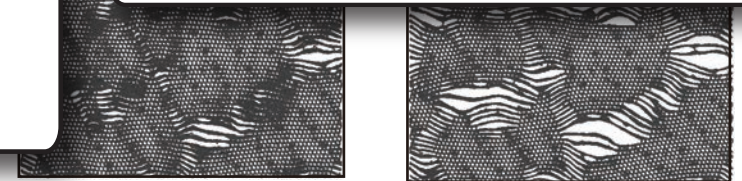
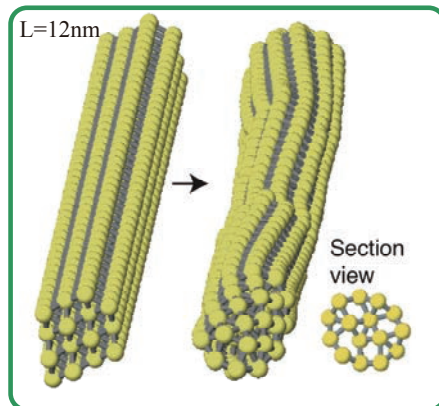
## Amourphous-like conjugated polymer (poly-(9,9 dioctyl fluorene))



Recent paper :

T. Hoshi, S. Yamamoto,  
T. Fujiwara, T. Sogabe,  
S-L Zhang, J. Phys.: CM 24,  
165502 (2012) ;  
(Acknowl. : M. Ishida  
(Sumitomo Chemical Co.) )

## helical gold nanowire



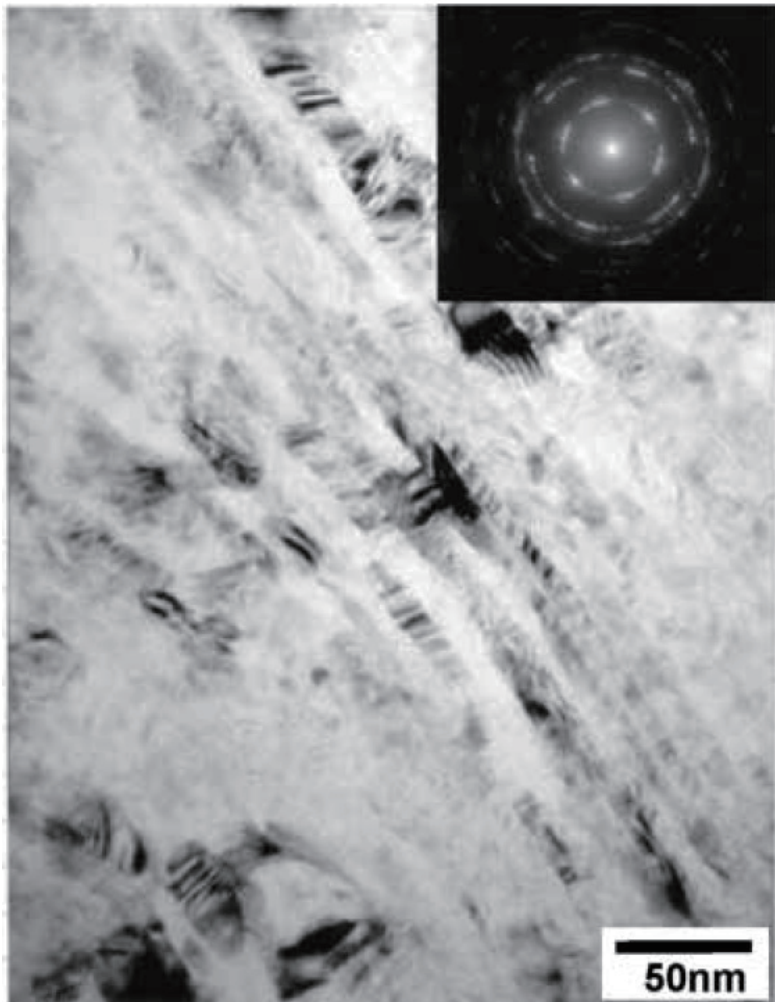
# Nano-polycrystalline diamond (NPD)

→ novel ultra-hard material

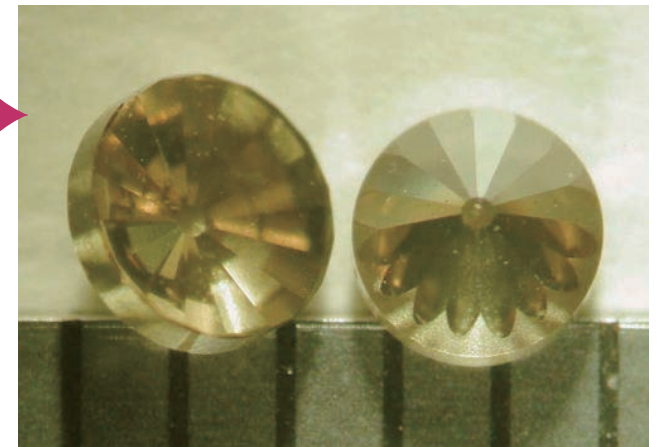
T. Irifune, et al. , Nature 421, 599 (2003) (@ Ehime Univ. )

→ harder than conventional diamond crystals

100-nm-scale structure



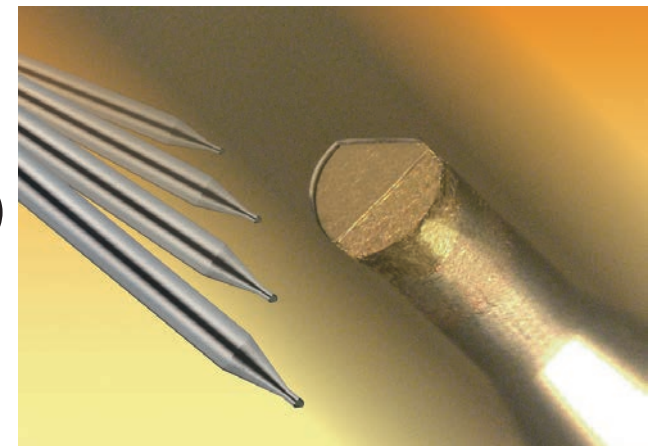
macroscale  
sample



1 mm



industrial product (2012)  
(Sumitomo Electric  
Industries )



# Visualization analysis on $sp^2$ / $sp^3$ nano composite carbon solid

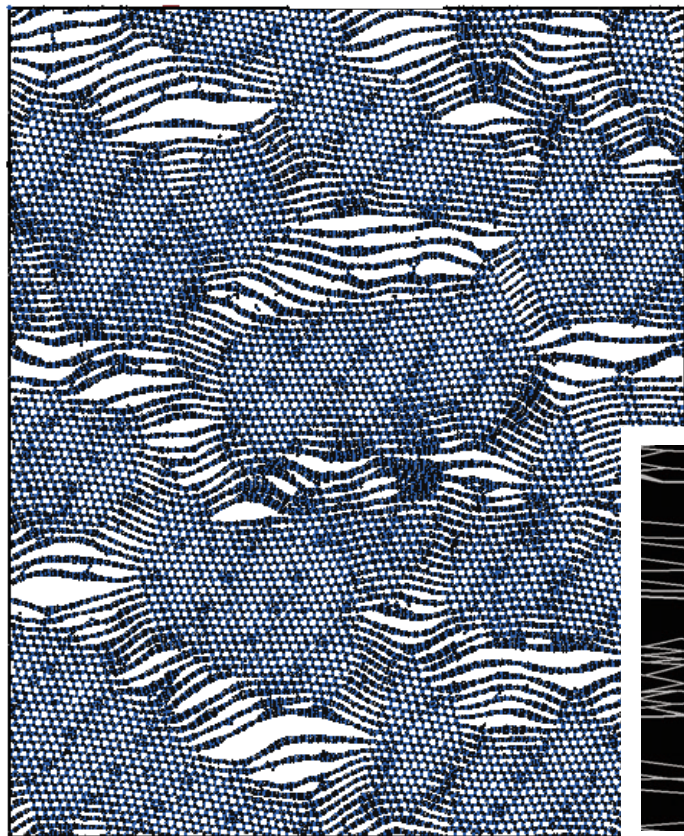
- Preliminary research for nano-polycrystalline diamond
  - (1) Massively parallel quantum molecular dynamics
  - (2) Massively parallel Green's function analysis ( $\pi$ -COHP\*)

→ the distinction between  $sp^2$  and  $sp^3$ -domains

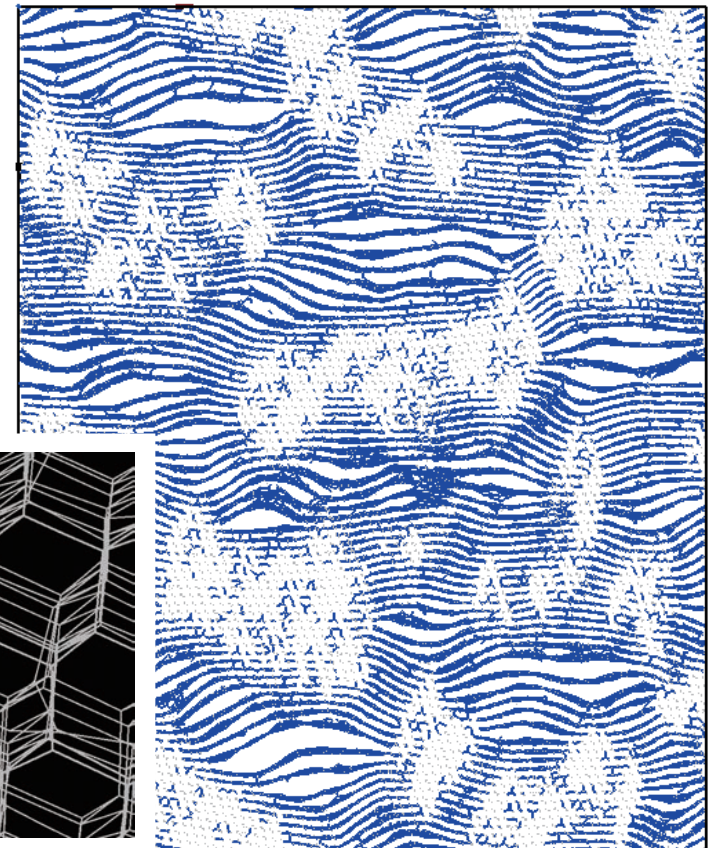
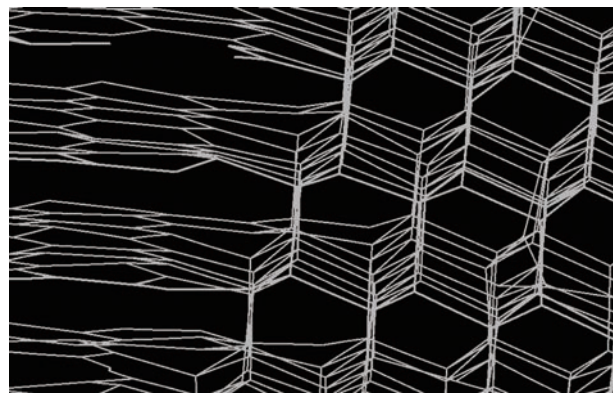
(A) Visualize  $sp^2$  and  $sp^3$  domains

(B) Visualize only  $sp^2$  domains

← 17 nm →



$sp^2$ - $sp^3$   
domain  
boundary



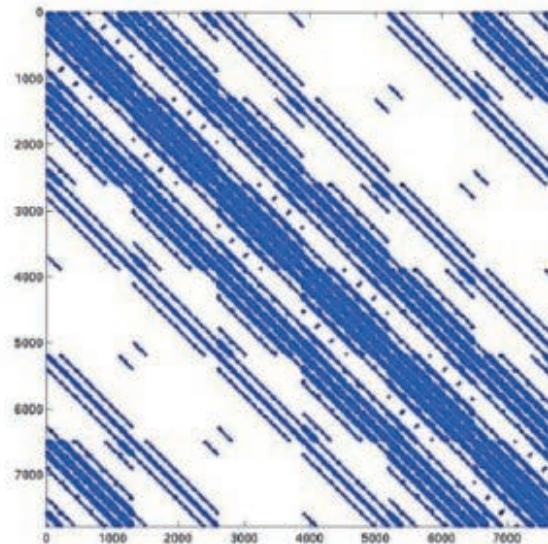
# 'Open data' of sparse matrices

→ A possible 'seed' for further collaboration between mathematics and physics

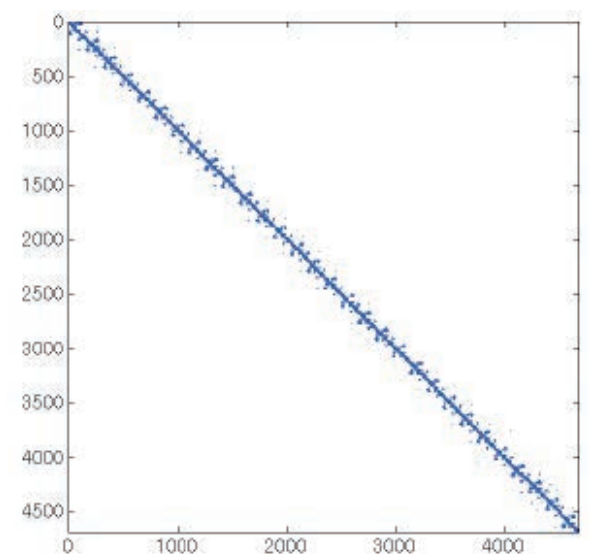
ELSES matrix library :  
<http://www.elses.jp/matrix/>

( various matrix sizes  
upto 1 M)

Solid  
(gold)



Polymer  
(poly-fluorene)



cf. similar site: Matrix Market ( <http://math.nist.gov/MatrixMarket/> )

# Summary

- Numerical linear algebra plays a crucial role in Application-Algorithm-Architecture co-design among (post-)peta-scale calculations
  - Krylov-subspace solvers for generalized shifted linear equation

$$(zS - H)x = b$$

in stead of conventional generalized eigen-value equation

- Massively parallel computation, with upto all cores of the K computer
  - one-hundred-million-atom electronic structure calculation
  - 100-nm-scale systems, such as nano-polycrystalline diamond
- ‘Open data’ of sparce matrices ( <http://www.elses.jp/matrix/> )
  - possible seed for further collaboration



# Basic equations

Generalized eigen-value (GEV) equation

$$H \mathbf{y}_k = \varepsilon_k S \mathbf{y}_k$$

$H, S$  : Hermitian,  $S$ : positive definite ( $S \doteq I$ )

wavefunction  
formulation

$$G = \sum_k \frac{\mathbf{y}_k \mathbf{y}_k^T}{z - \varepsilon_k}$$

Generalized shifted linear (GSL) equations

$$(zS - H) \mathbf{x} = \mathbf{b} \quad (z : \text{complex energy})$$

non-Hermitian

$$\rightarrow \mathbf{x} = G \mathbf{b}$$

with  $G \equiv (zS - H)^{-1}$  : the Green's function

the propagation  
(Green's) function  
formulation



# Physical quantities in trace form

Generalized eigen-value problem

$$H\mathbf{y}_k = \varepsilon_k S\mathbf{y}_k \quad (1)$$

Physical quantity in a trace form:

(Ex. the case of  $X=H$

--> Electronic structure energy)

$$\begin{aligned} \langle X \rangle &\equiv \sum_k f_k \mathbf{y}_k^t X \mathbf{y}_k \\ &= \text{Tr}[\rho X] \end{aligned} \quad (2)$$

with the one-body density matrix

$$\rho \equiv \sum_k f_k \mathbf{y}_k \mathbf{y}_k^t \quad (3)$$

Decomposition of the trace form

$$\text{Tr}[\rho X] = \sum_j \underbrace{\mathbf{e}_j^t \rho X \mathbf{e}_j}_{\text{red wavy line}} \quad (4)$$

with  $\mathbf{e}_j$  (j-th unit vector)

$$\mathbf{e}_j \equiv (0, \dots, 0, 1_j, 0, \dots, 0)^t \quad (5)$$



**“projected physical quantity”  
( to be calculated )**