超大規模電子状態計算コードELSESの紹介
- NIMSソフトウェアとの連携研究可能性 –

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1, Overview

- Application-Algorithm-Architecture co-design -

2, ELSESの紹介(「京」でのベンチマークも)

3, アルゴリズム(基本部分のみ)

4, Post-calculation analysis

5, 応用研究例

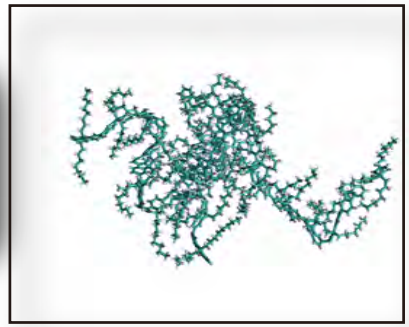
DFT-PW計算との連携研究など

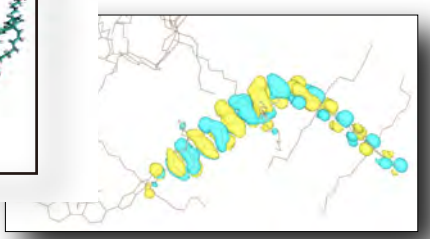
6, Conclusion - Material researchにおける2つの連携軸-

Overview : Application-Algorithm-Architecture co-design

a common concept in the current computational physics

Application : Materials research with electronic structure





Algorithm : Numerical linear algebra

$$H\boldsymbol{y} = \lambda S\boldsymbol{y}$$

$$(zS - H)\boldsymbol{x} = \boldsymbol{b}$$

Architecture : from top-class supercomputers to small (personal) computers

http://www.elses.jp

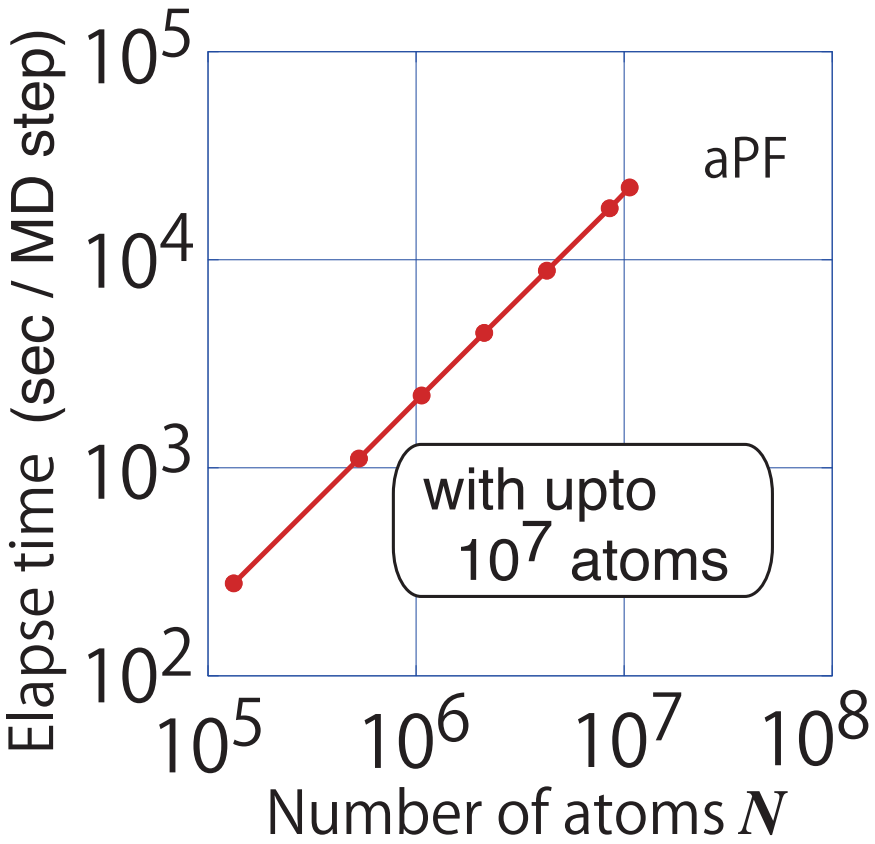
'ELSES' : Our code for 'order-*N*' electronic structure calculations

Hoshi et al.,JPCM24, 165502 (2012); Hoshi et al., Preprint (arXiv:1210.1531).

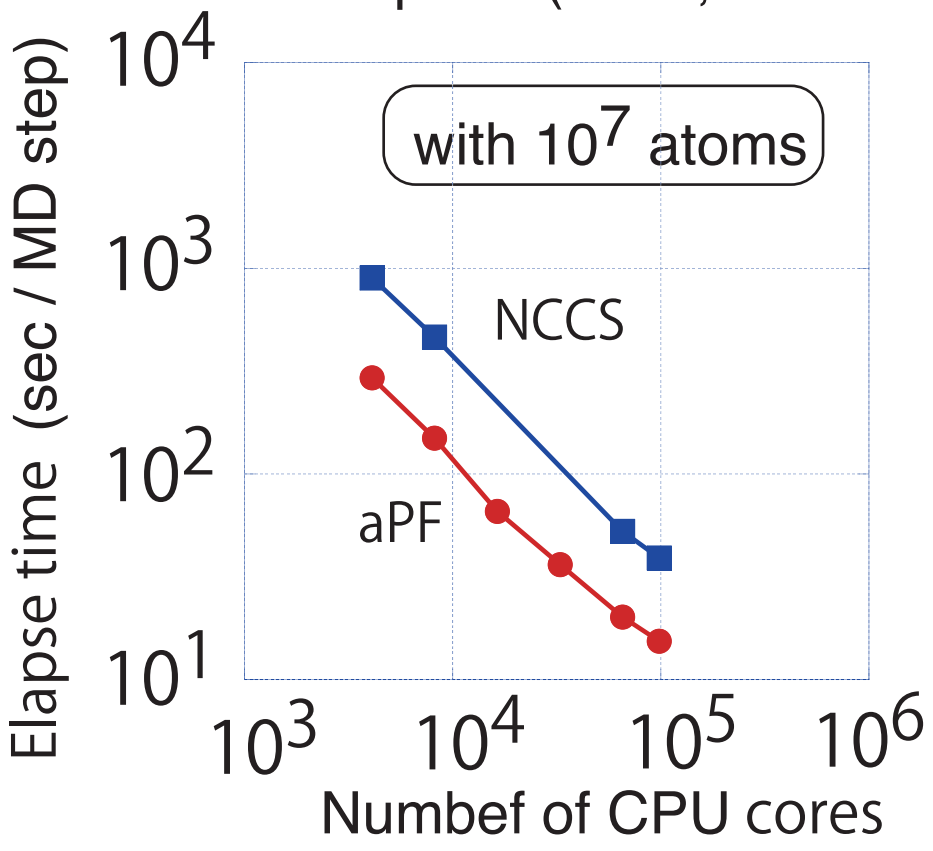
Benchmark with nanomaterials(~10^7 atoms) (cf. 10^7 atoms ~ Si : $(70\text{nm})^3$region)

aPF :amourphous-like conjugated polymer, poly-(9,9 dioctil-fluorene),
NCCS: sp2-sp3 nano composite carbon solid

(a) Order-*N* scaling



(b) Parallel efficiency (strong scaling)
on the K computer (~ 98,304 cores)



http://www.elses.jp/

大規模電子状態計算コード「ELSES」の紹介

ELSES(=Extra-Large-Scale Electronic Structure calculation)

謝辞

現在の予算的補助

・JST-CREST

領域「ポストペタスケール高性能計算に資するシステムソフトウェア技術の創出」

・JST-ASTEP(シーズ育成タイプ)

「ナノスケール材料向け超大規模電子構造計算プログラムの実用化研究開発」

・科研費新学術領域「 コンピューティクスによる物質デザイン」

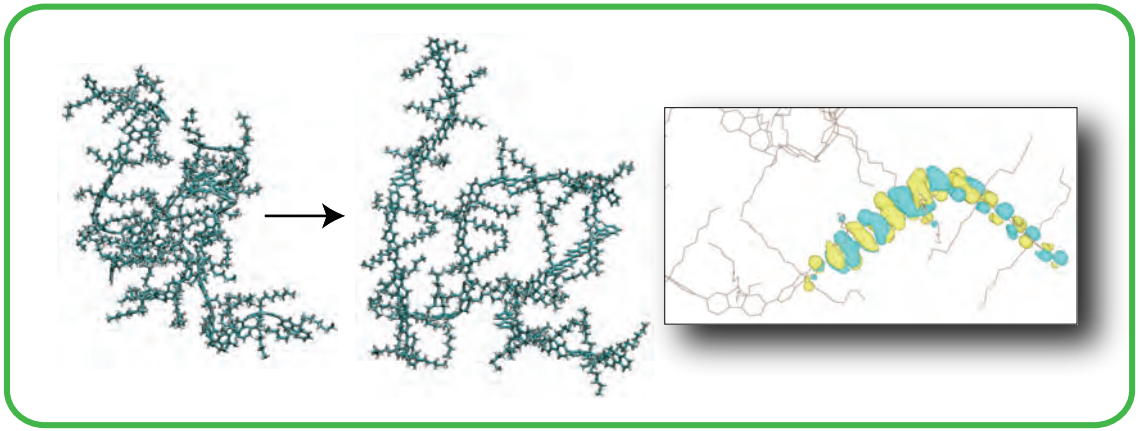
・その他

本発表における「京」利用の謝辞

・本研究の一部はHPCI戦略プログラム分野４(次世代ものづくり)の補助を受け実施した。
本結果の一部は、理化学研究所が実施している京速コンピュータ「京」の試験利用による。

Examples of nano-material studies with 'ELSES'

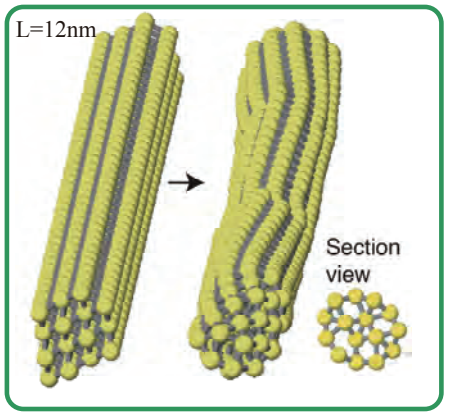
Amourphous-like conjugated polymer



Motivations

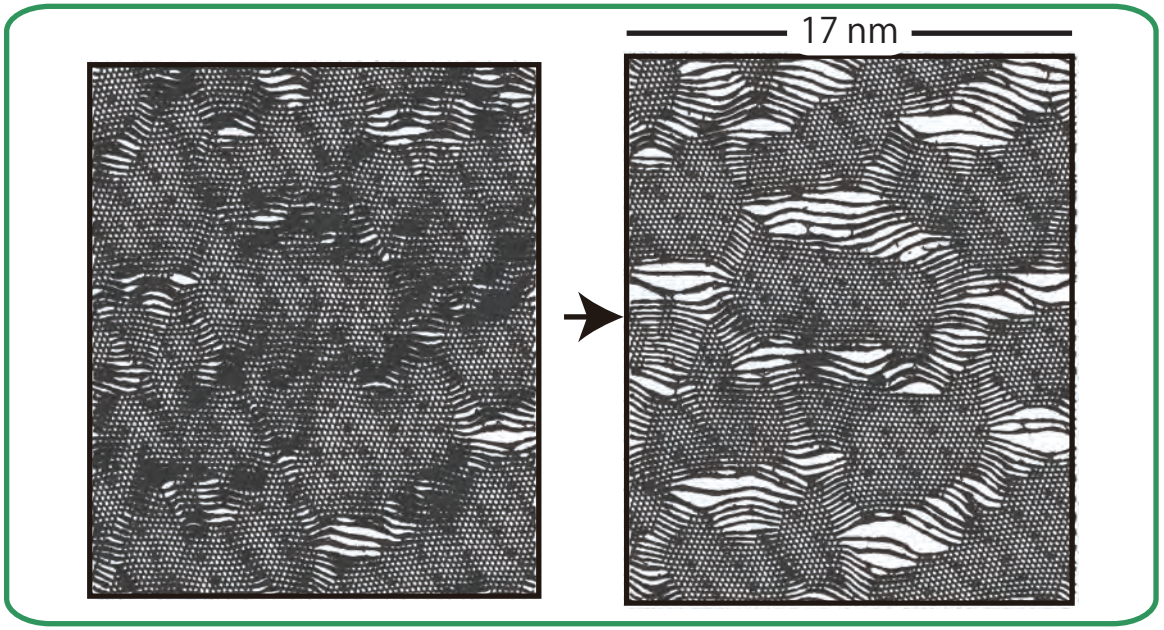
(i) for industrial application
(ii) new material (from Japan)
(iii) standard material

helical gold nanowire

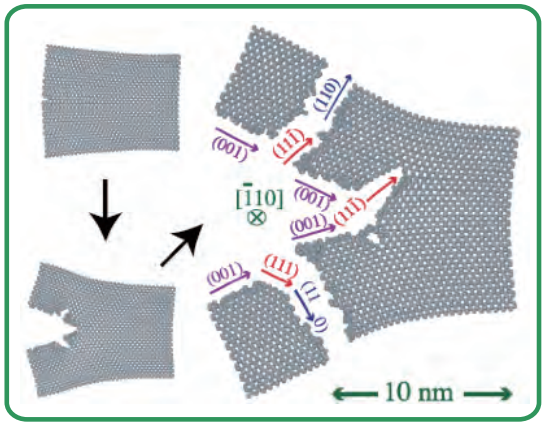


sp2-sp3 nano-composite carbon solid

(in research of nano-polycrystalline diamond)



silicon brittle fracture



Krylov subspace solver

... is the general name of iterative solvers,

such as CG algorithm for $A\boldsymbol{x} = \boldsymbol{b}$ $(A : \text{Hermitian})$

- Solvers for sparce matrices
- Mathematical foundation of order-N calculations

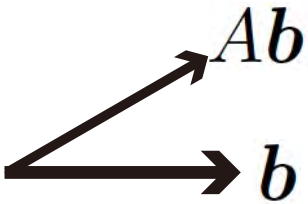
'projection' on the Krylov subspace of

$$K_n(A; \boldsymbol{b}) \equiv \text{span}\left\{\boldsymbol{b}, A\boldsymbol{b}, A^2\boldsymbol{b}, ..., A^{n-1}\boldsymbol{b}\right\}$$

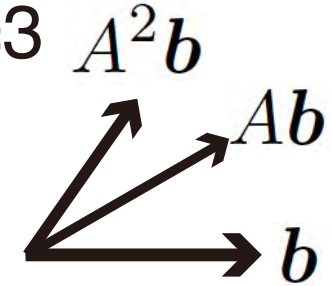
n : subspace dimension (iteration number)

n =1

n =2



n=3



Basic equations

Generalized eigen-value equation

wavefunction formulation

$$H\boldsymbol{y} = \varepsilon S\boldsymbol{y}$$

H, S : Hermitian ($\in R^{MxM}$), S: positive definite ($S \fallingdotseq I$)

Generalized shifted linear equations

the Green's function formulation

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

non-Hermitian

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

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

Six novel Krylov subspace solvers

Teng *et al*. PRB83, 165103 (2011); Yamashita *et al*.,Trans of JSIAM 21, 241 (2011); Hoshi *et al*.., JPCM 24, 165502 (2012). Sogabe *et al*., J. Comp. Phys. 231, 5669 (2012)

$$(zS - H)\boldsymbol{x} = \boldsymbol{b}$$ (generalized shifted linear equations)

classification by the solver principles

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

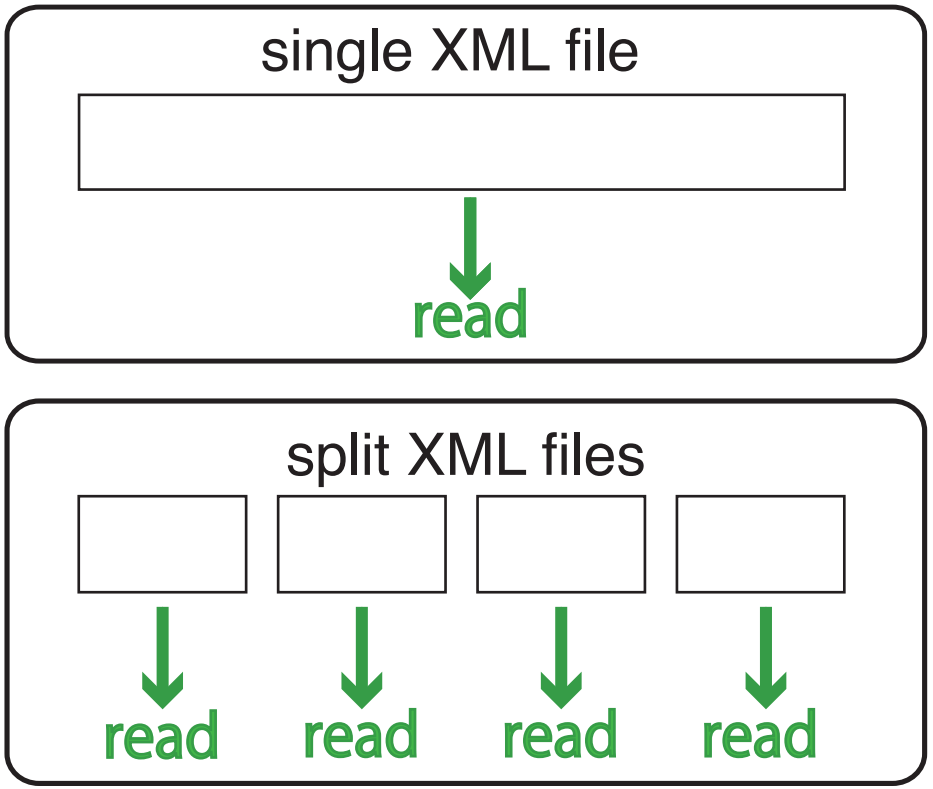
(*)Takayama *et al*., JPSJ73, 1519 (2004); Takayama et al. PRB 73, 165108(2006); Sogabe et al. ETNA31, 126 (2008)

File-IO issue : Parallel file reading with split XML file

ex. Acceralation in the initial procedure with 10M atoms

(a) with non-parallel file reading
→ T =1426.6 sec

(b) with parallel file reading
→ T = 69.6 sec



NOTE: XML parsers (file-reading method)

- DOM(object based) → impractical for large data
- SAX (stream based) → good for large data (used)

Post-calculation analysis method

.....is crucial, so as to obtain physical conclusions from huge electronic-structure data

Large-scale calculation
by massively-parallel computers

↓

Huge elctronic structure data
(as the Green's function)

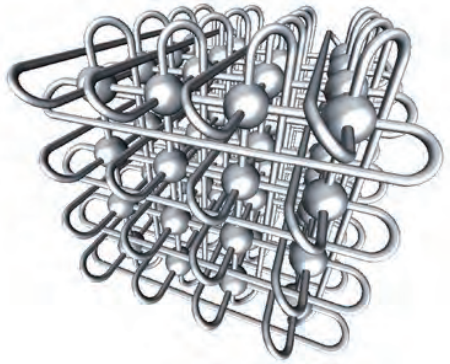
↓

Post-calculation analysis

↓

Physical conclusions

distributed among nodes



ex. (π)COHP analysis
→next page

Crystal Orbital Hamiltonian Population(COHP) analysis

*Dronskowski and Blochl, J. Phys. Chem. 97, 8617 (1993).

→ Local bond energy analysis,
based on the Green's functions

COHP for (I, J) atom pair

$$C_{IJ}(\varepsilon) \equiv \frac{-1}{\pi} \sum_{\alpha\beta} H_{J\beta,I\alpha} \operatorname{Im} G_{I\alpha,J\beta}(\varepsilon + i0) \quad (1)$$

(α, β : orbitals)

Integrated COHP (I-COHP)

$$B_{IJ} \equiv \int^{\varepsilon_F} C_{IJ}(\varepsilon) d\varepsilon \quad (2)$$

(Sum of the ICOHP) = (elec. str. energy)

$$E_{\text{elec}} \equiv \sum_k f_k \varepsilon_k = \sum_{I,J} B_{IJ} \quad (3)$$

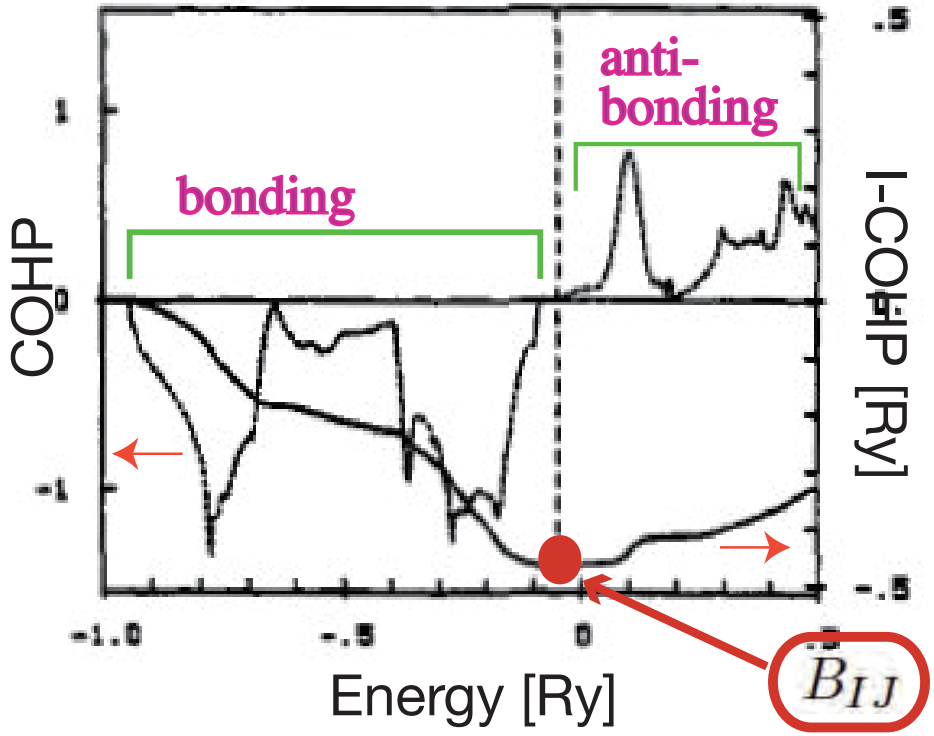
Decomposition into σCOHP and πCOHP**

$$C_{IJ}(\varepsilon) = C_{IJ}^{(\sigma)}(\varepsilon) + C_{IJ}^{(\pi)}(\varepsilon) \quad (I \neq J) \quad (4)$$

with sp orbitals

**T. Hoshi et al., Preprint (arXiv:1210.1531)

Ex. Si crystal (*ab initio* (LMTO) calc.)*



Crystal Orbital Hamiltonian Population(COHP) analysis

*Dronskowski and Blochl, J. Phys. Chem. 97, 8617 (1993).

→ Local bond energy analysis,
based on the Green's functions

COHP for (I, J) atom pair

$$C_{IJ}(\varepsilon) \equiv \frac{-1}{\pi}$$

Integrated C

$$B_{IJ}$$

(Sum of the

$$E_{\mathrm{elec}} \equiv \sum_k f_k \varepsilon_k = \sum_{I,J} B_{IJ} \qquad (3)$$

Decomposition into σCOHP and πCOHP**

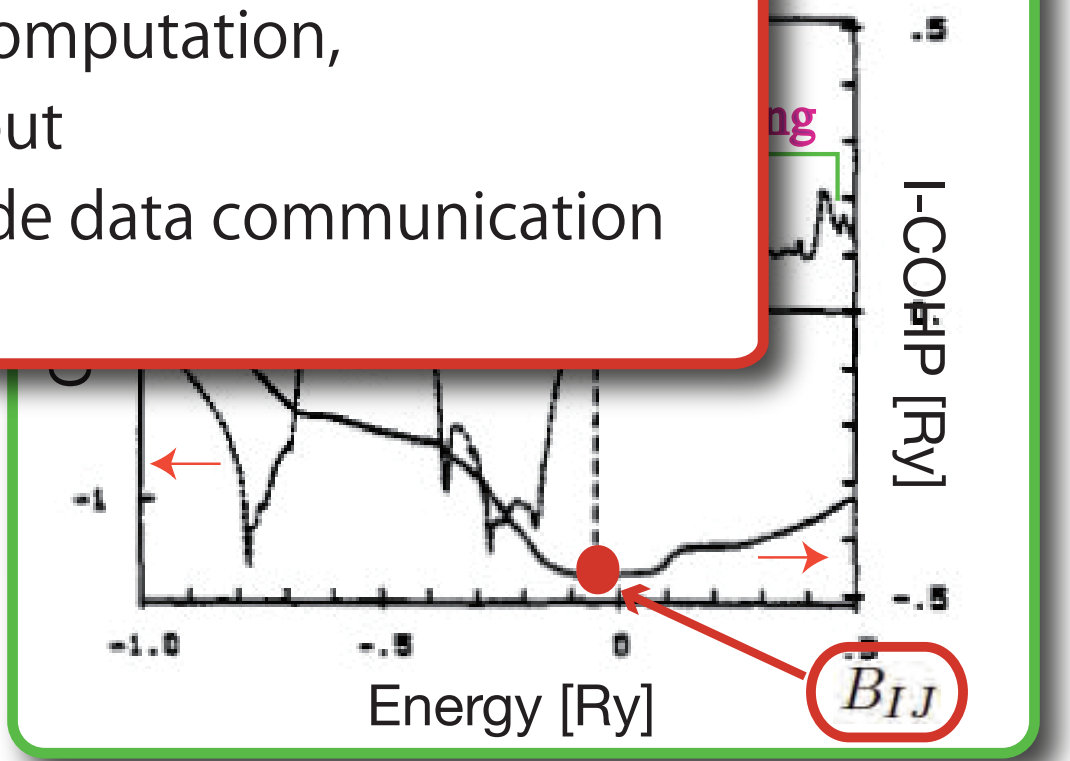
$$C_{IJ}(\varepsilon) = C_{IJ}^{(\sigma)}(\varepsilon) + C_{IJ}^{(\pi)}(\varepsilon) \quad (I \neq J) \qquad (4)$$

with sp orbitals

v:1210.1531)

Remarks :
the (σ, π)COHP analysis is ideal for
a massively parallel computation,
because it is carried out
without any inter-node data communication

) calc.)*



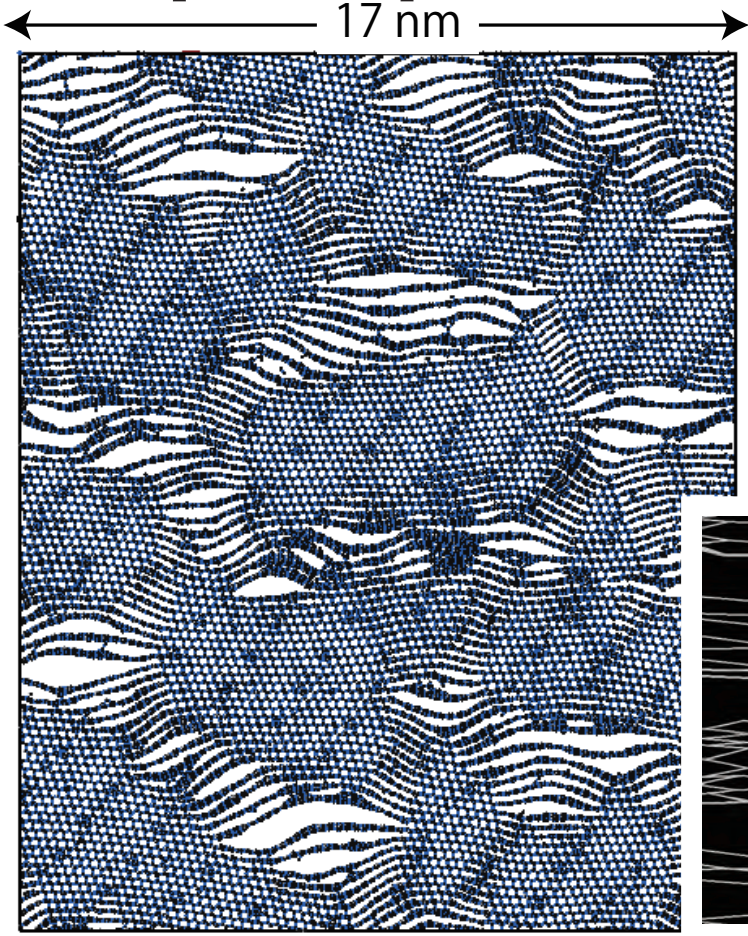
Example of post-calculation large-data analysis by (π)COHP analysis

Visualization analysis in sp2-sp3 nano-composite carbon solids

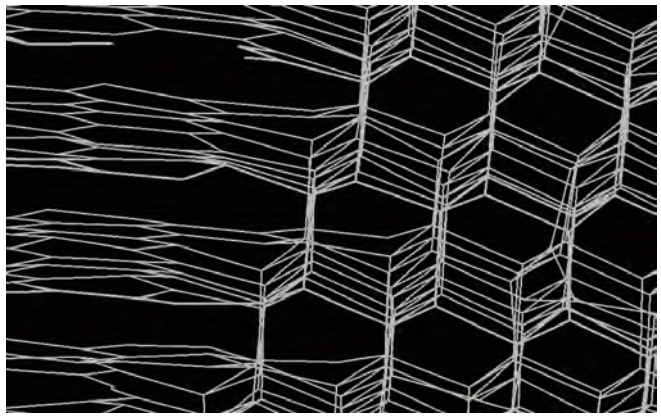
Hoshi et al, Preprint (arXiv:1210.1531)

result of a MD simulation with 100K atoms
→ distinction of sp2 and sp3 domains

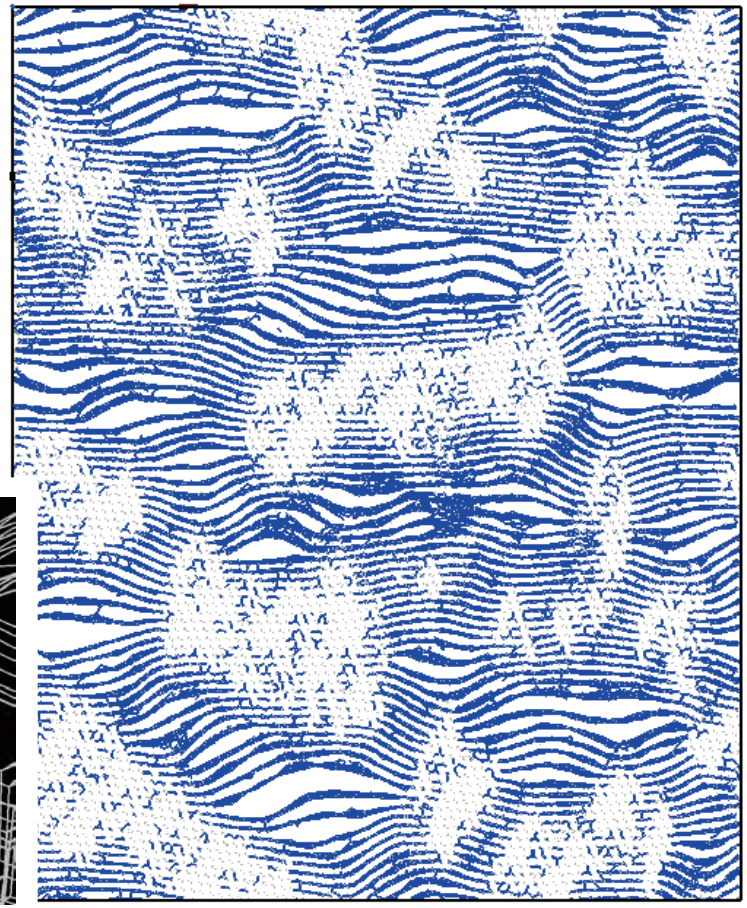
(a) Visualization
for sp2 and sp3 domains



sp2-sp3 domain
boundary ↓



(b) Visualization
only for sp2 domains



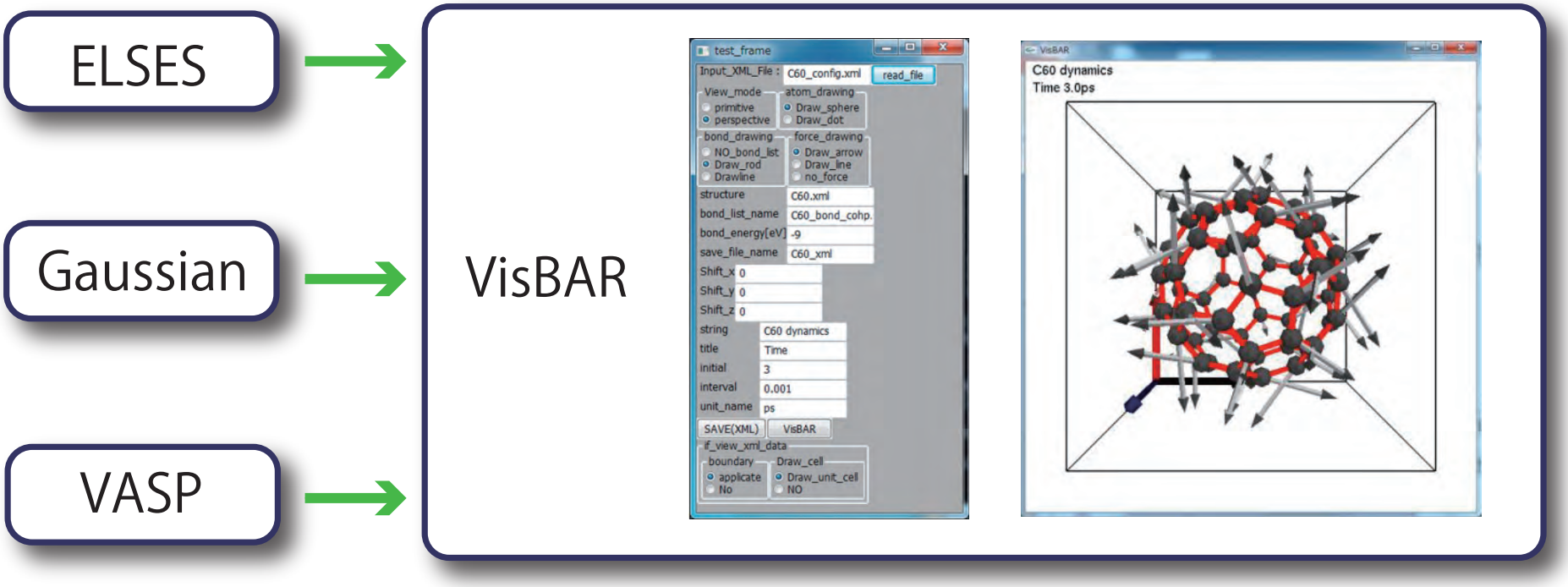
Original python-based visualization tool ‘VisBAR’

→ Python + XML+ OpenGL (3D) + wxPython (GUI, optional)

Motivations

1, Our special needs arising from large-scale calculation,
such as bond visualization by (π) COHP analysis

2, Cooperative research with different simulation softwares
→ ELSES / Gaussian / VASP.



http://www.elses.jp

Ten-million-atom electronic structure calculations with novel linear-algebraic algorithm and the K computer

Latest preprint (arXiv:1210.1531)

summary (partial)

1. Overview
   - Application-Algorithm-Architecture co-design
2. Benchmark and applications
   - parallel efficiency ('strong scaling') on the K computer for ten-million-atom materials with 100K CPU cores
   - application to nanomaterial research (brief)
3. Algorithm
   - Krylov subspace solver for generalized shifted linear equatons
     → the Green's function formulation
   - memory-saving workflow
4. Post-calculation analysis method
   - (π)COHP analysis, suitable for parallelism
     → example in sp2-sp3 nano-compsite carbon solids

マルチスケール電子状態計算

T.Hoshi et al., PRB72, 075323 (2005); Physica E42, 2784 (2010).

シリコン脆性破壊に現れるステップ構造の理論的予言と解析

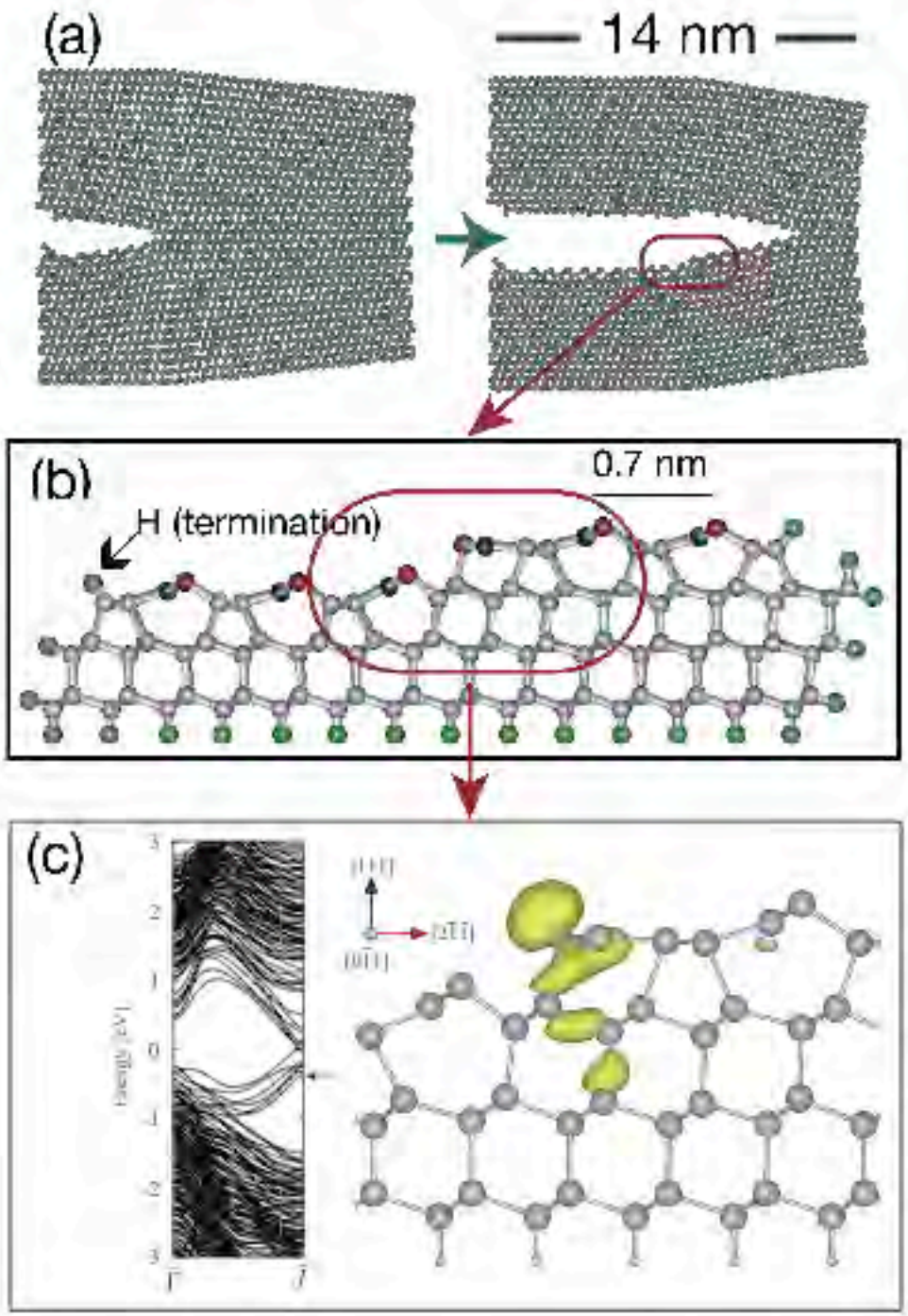
(a) 超大規模計算(ELSES)
10nm-scale系, へき開プロセス(~10ps)
→特徴的6員環ステップ構造の出現(理論的予言)

↓ 高精度(小規模)計算での解析

(b) 高精度第一原理(DFT+PW)計算(VASP*)
ステップ端付近の「close-up」構造
→2種のチルト構造
(higher energy構造, lower energy構造)
→(エネルギーバリア)~0.2 eV
Nudged Elastic Band (NEB)計算

(c) ステップ端の波動関数
→バイアス依存型STM像(予想)

*http://www.vasp.at/



Iguchi, Hoshi, Fujiwara, PRL99, 125507 (2007); T. Hoshi and T. Fujiwara, JPCM 21, 272201 (2009)

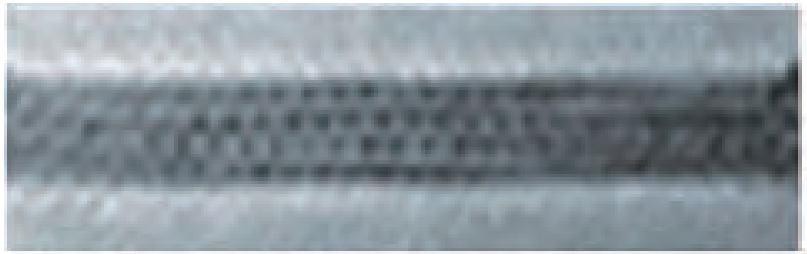
Helical multishell gold nanowires

Invited review article: Hoshi, Iguchi, Fujiwara, Sec. 18 of 'Handbook of Nanophysics 4', CRC Press (2010)

Experiment

Kondo and Takayanagi,
Science **289**, 606 (2000).

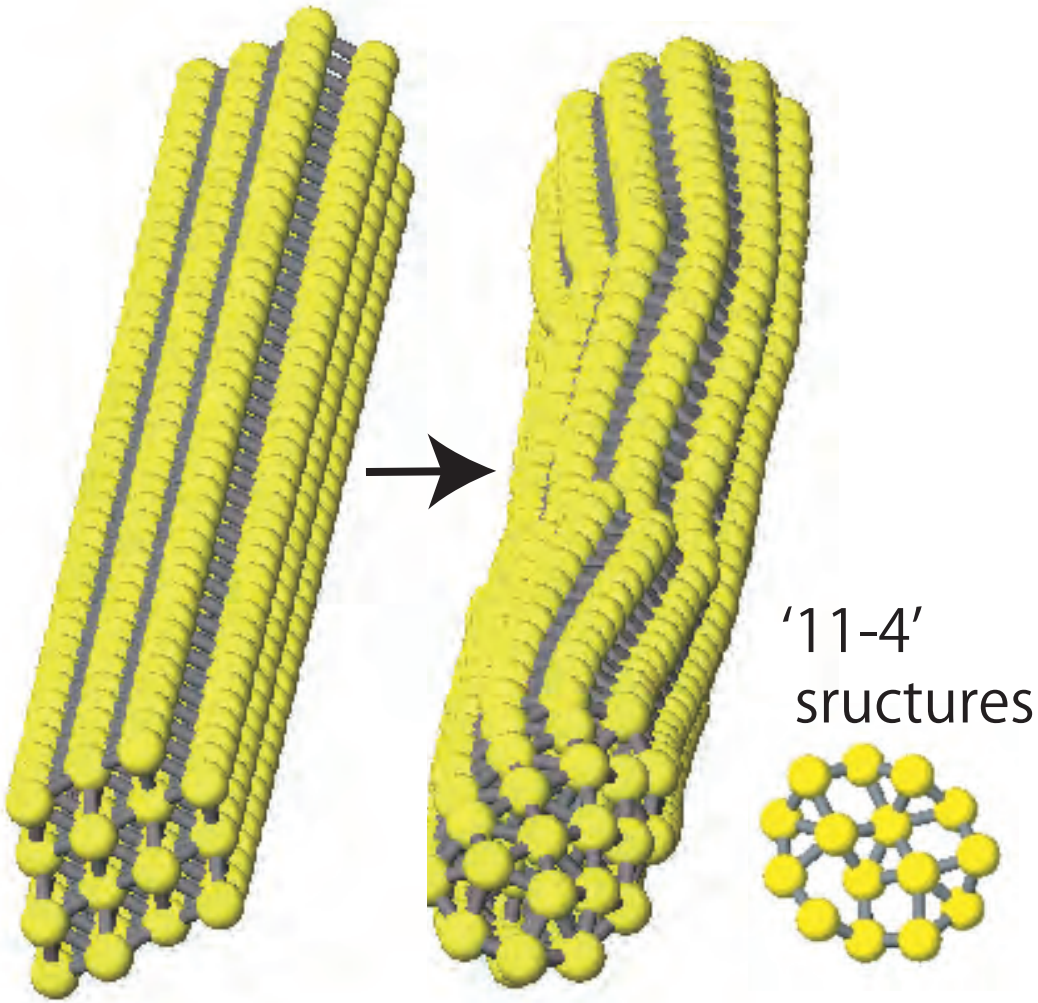
ex. TEM image of 11-4 structure



→ Specific shell configurations with "magic number"

: 7-1, 11-4, 13-6, 14-7-1, 15-8-1 structures

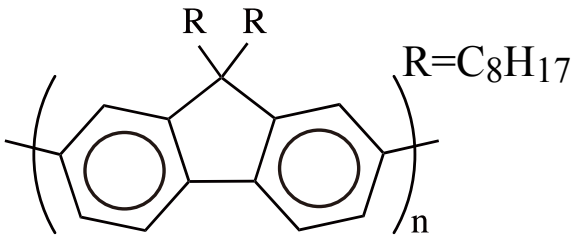
Theory and simulation

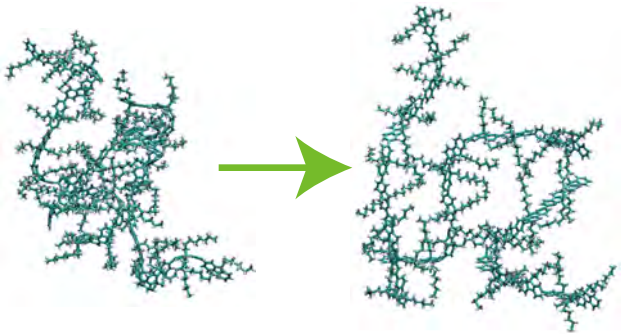


amourphous-like conjugated polymer, poly-(9,9 dioctyl-fluorene)

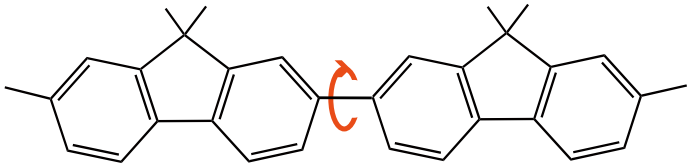
An early-stage research

→ characteristic localized π states over two or three monomers because of the twisting between monomers

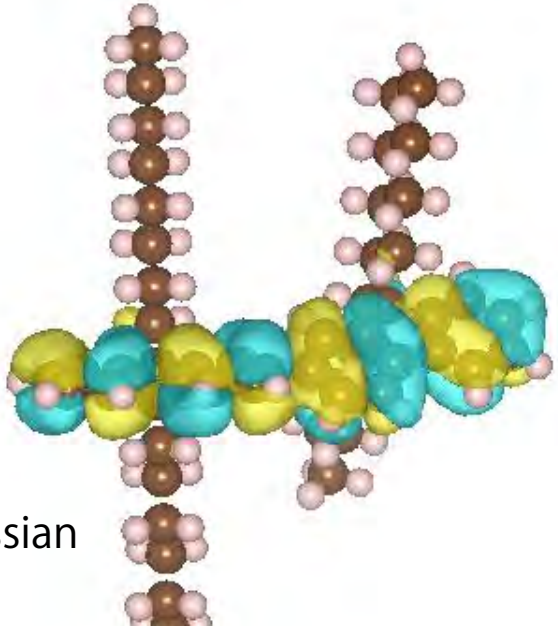




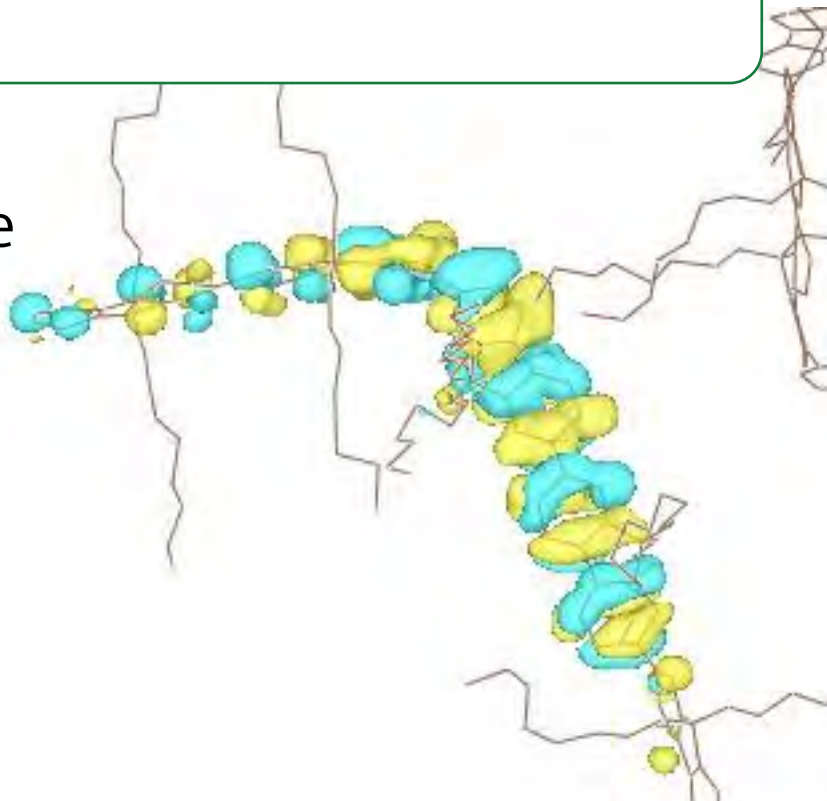
Twisting freedom



HOMO in dimer



HOMO in amourphous-like structure



ELSES and Gaussian

Conclusion : Materials researchにおける2種類の連携軸