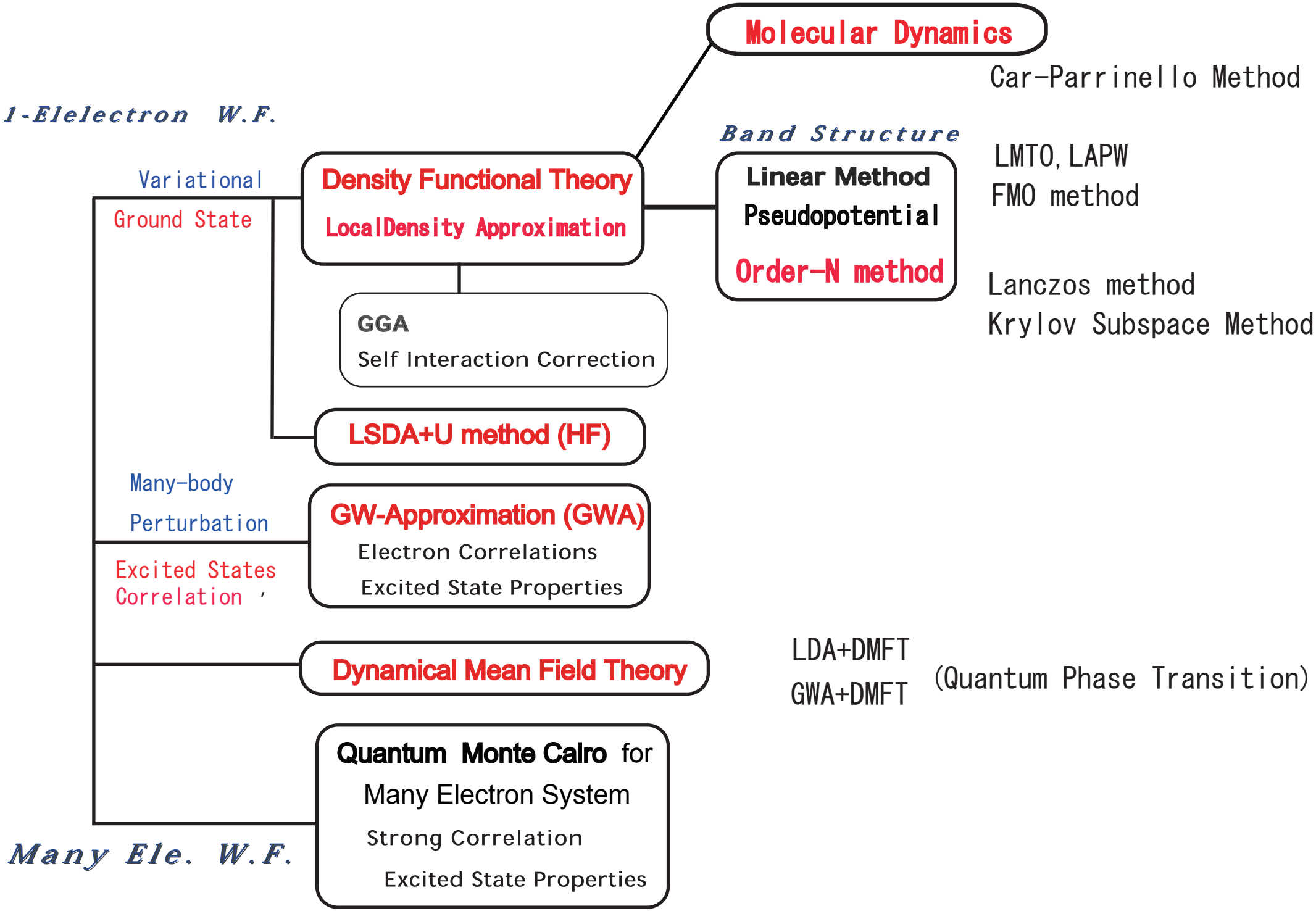
2007年2月28日　最終講義

固体電子構造理論について

東京大学工学系研究科物理工学専攻

藤原毅夫

‡：このマークが付してある著作物は、第三者が有する著作物ですので、同著作物の再使用、
同著作物の二次的著作物の創作等については、著作権者より直接使用許諾を得る必要があります。


Molecular Dynamics
Car-Parrinello Method
1-Elelectron W.F.
Band Structure
Variational
Ground State
Density Functional Theory
LocalDensity Approximation
Linear Method
Pseudopotential
Order-N method
LMTO, LAPW
FMO method
Lanczos method
Krylov Subspace Method
GGA
Self Interaction Correction
LSDA+U method (HF)
Many-body
Perturbation
GW-Approximation (GWA)
Electron Correlations
Excited State Properties
Excited States
Correlation
Dynamical Mean Field Theory
LDA+DMFT
GWA+DMFT
(Quantum Phase Transition)
Quantum Monte Calro for
Many Electron System
Strong Correlation
Excited State Properties
Many Ele. W.F.

PHYSICAL REVIEW VOLUME 136, NUMBER 3B 9 NOVEMEBR 1964

Inhomogeneous Electron Gas*

P. HOHENBERG†
École Normale Superieure, Paris, France
AND
W. KOHN‡
École Normale Superieure, Paris, France and Faculté des Sciences, Orsay, France
and
University of California at San Diego, La Jolla, California

‡

$$Q[n_\uparrow, n_\downarrow] = \underset{\Psi \in \{n_\uparrow n_\downarrow\}}{\mathrm{Min}} \langle \Psi_{n_\uparrow n_\downarrow} | \hat{T} + \hat{V}_{e-e} | \Psi_{n_\uparrow n_\downarrow} \rangle$$

$Q[n_\uparrow, n_\downarrow]$:電子密度のユニバーサルな汎関数

$$E_{DTF}[n_\uparrow, n_\downarrow] \equiv Q[n_\uparrow, n_\downarrow] + \int d\boldsymbol{r} w_{ext}(\boldsymbol{r}) n(\boldsymbol{r}) \geq E_{g.s.}$$

$$n(\boldsymbol{r}) = n_\uparrow(\boldsymbol{r}) + n_\downarrow(\boldsymbol{r})$$

$$\begin{aligned} E_{DTF}[n_\uparrow, n_\downarrow] &= T[n_\uparrow, n_\downarrow] + E^{e-e}[n_\uparrow, n_\downarrow] + \int d\boldsymbol{r} w_{ext}(\boldsymbol{r}) n(\boldsymbol{r}) \ . \\ &= T_0[n_\uparrow, n_\downarrow] + U[n] + E_{xc}[n_\uparrow, n_\downarrow] + \int d\boldsymbol{r} w_{ext}(\boldsymbol{r}) n(\boldsymbol{r}) \end{aligned}$$

$T_0[n_\uparrow, n_\downarrow]$:同じ電子密度を持った相互作用のない系の運動エネルギー

$$U[n] = \frac{1}{2} \int d\boldsymbol{r} d\boldsymbol{r}' \frac{n(\boldsymbol{r}) n(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|}$$

PHYSICAL REVIEW VOLUME 140, NUMBER 4A 15 NOVEMBER 1965

Self-Consistent Equations Including Exchange and Correlation Effects*

W. KOHN AND L. J. SHAM
University of California, San Diego, La Jolla, California
(Received 21 June 1965)



‡

$$n_\sigma(\boldsymbol{r}) = \sum_\alpha f_{\alpha\sigma} |\psi_{\alpha\sigma}(\boldsymbol{r})|^2$$

$$f_{\alpha\sigma} = 0,\ 1$$

$$T_0[\{f_{\alpha\sigma}, \psi_{\alpha\sigma}\}] = \sum_{\alpha\sigma} f_{\alpha\sigma} \langle \psi_{\alpha\sigma} | -\frac{1}{2}\Delta | \psi_{\alpha\sigma} \rangle$$

‡

$$\left[-\frac{1}{2}\Delta + v^\sigma_{eff}(\boldsymbol{r})\right]\psi_{\alpha\sigma}(\boldsymbol{r}) = \varepsilon_{\alpha\sigma}\psi_{\alpha\sigma}(\boldsymbol{r})\ .$$

$$v^\sigma_{eff}(\boldsymbol{r}) = w_{ext}(\boldsymbol{r}) + \int d\boldsymbol{r}' \frac{n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} + \frac{\delta E_{xc}[n_\uparrow, n_\downarrow]}{\delta n_\sigma(\boldsymbol{r})} = w_{ext}(\boldsymbol{r}) + v_H(\boldsymbol{r}) + \mu^\sigma_{xc}(\boldsymbol{r})$$

$$\frac{\partial}{\partial f_{\alpha\sigma}} E_{DFT} = \varepsilon_{\alpha\sigma}$$

「ヤナック (Janak) の定理」

$$E_{DFT} = \sum_{\alpha\sigma} f_{\alpha\sigma}\varepsilon_{\alpha\sigma} - \frac{1}{2}\int d\boldsymbol{r} \int d\boldsymbol{r}' \frac{n(\boldsymbol{r})n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} + E_{xc}[n_\uparrow, n_\downarrow] - \sum_\sigma \int d\boldsymbol{r} n_\sigma(\boldsymbol{r})\mu^\sigma_{xc}(\boldsymbol{r})$$

JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN Vol. 9, No. 5, SEP.—OCT., 1954

On the Absorption Spectra of Complex Ions. I

By Yukito TANABE
Department of Physics, University of Tokyo
and Satoru SUGANO
Institute of Broadcasting, N. H. K.
(Recieved June 11, 1954)

JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN Vol. 9, No. 5, SEP.—OCT., 1954

On the Absorption Spectra of Complex Ions II

By Yukito TANABE
Physics Department, Tokyo University
and Satoru SUGANO
Institute of Broadcating N.H.K.
(Received June 11, 1954)

‡



物理科学選書4

今井　功・小谷正雄・森野米三・永田　武・高橋秀俊 編集

配位子場理論とその応用

東京大学助教授 理学博士	東京大学助教授 理学博士	東京工業大学助教授 理学博士
上村　洸	菅野　暁	田辺行人

共　著

東京 裳 華 房 発行

‡

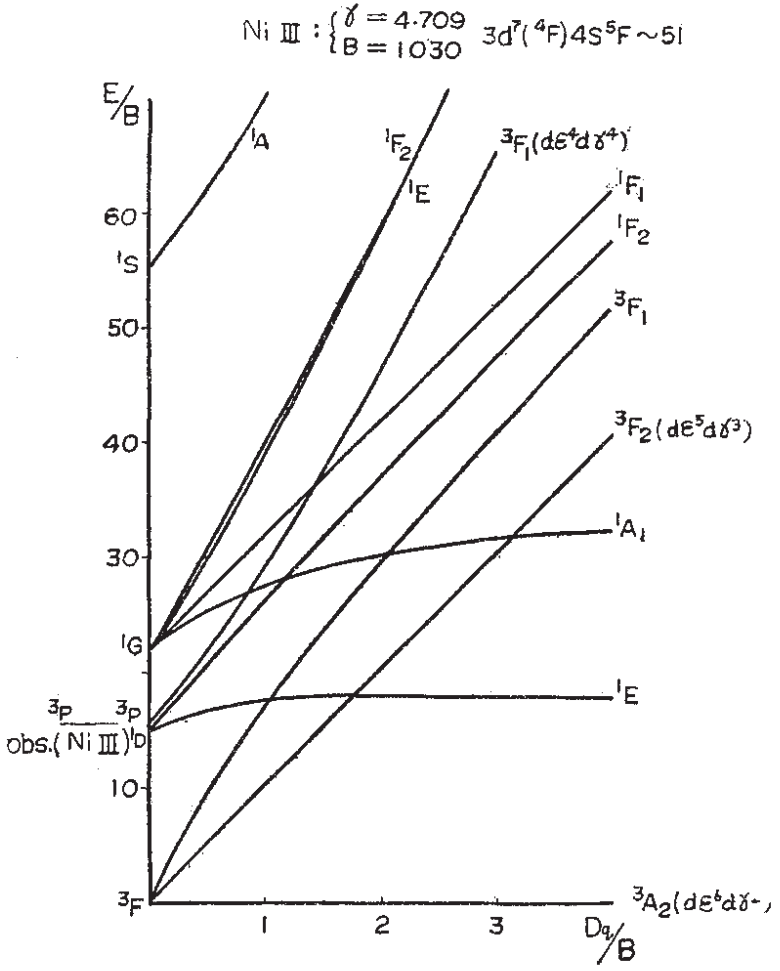


Fig. 4. The energy diagram for d^8. ‡

J. Phys. C: Solid State Phys., Vol. 5, 1972. Printed in Great Britain. © 1972

Electronic structure based on the local atomic environment for tight-binding bands

R HAYDOCK, VOLKER HEINE and M J KELLY
Cavendish Laboratory, Cambridge, UK

‡

Lanczos Method

Recursion Method

Gram-Schmidt の方法

$$|n+1\} = H|n\} - a_n|n\} - b_n|b-1\},$$
$$\{n|n+1\} = 0 \quad \rightarrow \quad \{n|m\} = 0 \quad (n \neq m)$$

$$\Rightarrow$$

$$\{n|H|n\} = a_n\{n|n\}, \quad \{n-1|H|n\} = b_n\{n-1|n-1\}$$

and

$$H_n \equiv \frac{\{n|H|n\}}{\{n|n\}},$$
$$H_{n-1,n} \equiv \frac{\{n-1|H|n\}}{\{n-1|n-1\}^{1/2}\{n|n\}^{1/2}},$$

$$\Rightarrow$$

$$H_{n,n} = a_n$$
$$H_{n-1,n} = H_{n,n-1} = [b_{n-1}]^{1/2}$$

$$\Rightarrow$$

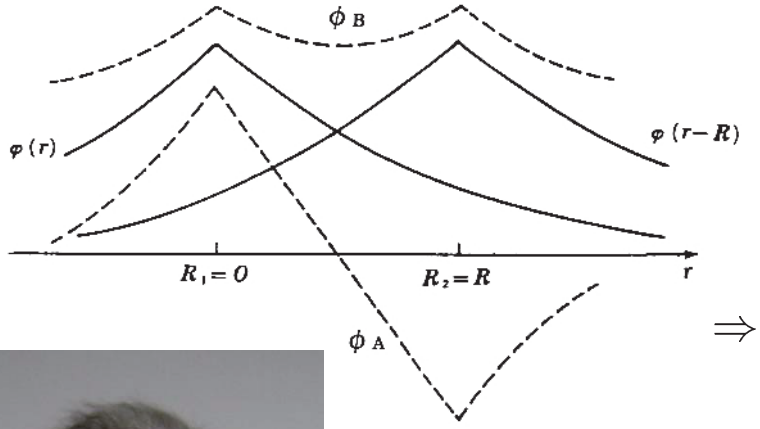
$$H = \begin{pmatrix} a_1 & b_1 & 0 & \cdots & & & \\ b_1 & a_2 & b_2 & 0 & \cdots & & \\ 0 & b_2 & a_3 & \ddots & \ddots & & \\ \vdots & 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ & \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ & & & \ddots & \ddots & \ddots & b_{N-1} \\ & & & \cdots & 0 & b_{N-1} & a_N \end{pmatrix}$$

PHYSICAL REVIEW B VOLUME 12, NUMBER 8 15 OCTOBER 1975

Linear methods in band theory*

O. Krogh Andersen
Department of Electrophysics, Technical University, Lyngby, Denmark

‡





‡

$$\phi_{B/A}(\boldsymbol{r}) = \phi_L(\boldsymbol{r}) \pm (-1)^l \phi_L(\boldsymbol{r}-\boldsymbol{R}),$$

$$\Rightarrow$$

$$\phi_L(\boldsymbol{r}) = \frac{1}{2}\{\phi_B(\boldsymbol{r}) + \phi_A(\boldsymbol{r})\},$$

$$\phi_L(\boldsymbol{r}-\boldsymbol{R}) = \frac{(-1)^l}{2}\{\phi_B(\boldsymbol{r}) - \phi_A(\boldsymbol{r})\}$$

$$\Rightarrow$$

$$\phi_L(\boldsymbol{r}) \cong \phi_{E_0}(\boldsymbol{r}) + c_1\dot{\phi}_{E_0}(\boldsymbol{r}),$$
$$\phi_L(\boldsymbol{r}-\boldsymbol{R}) \cong c_2\dot{\phi}_{E_0}(\boldsymbol{r}),$$

$$\Rightarrow$$

$$\chi_{\boldsymbol{R}L}(\boldsymbol{r}-\boldsymbol{R}) = \phi_{\boldsymbol{R}L}(\boldsymbol{r}-\boldsymbol{R}) + \sum_{\boldsymbol{R}'}\sum_{L'}\dot{\phi}_{\boldsymbol{R}'L'}(\boldsymbol{r}-\boldsymbol{R}')h_{\boldsymbol{R}'L':\boldsymbol{R}L}$$

(LMTO+Lanczos, 大規模系＋第一原理)

Journal of Non-Crystalline Solids 61 & 62 (1984) 1039-1048
North-Holland, Amsterdam

ELECTRONIC STRUCTURE CALCULATIONS FOR AMORPHOUS ALLOYS

!!!!削除!!!!

Takeo FUJIWARA

Max-Planck-Institut für Festkörperforschung, 7000 Stuttgart 80,
Federal Republic of Germany *

IS

We define the generalized, screened structure constant[15]

$$\bar{S} = S\,(1 - \bar{Q}^{-1}\,S)^{-1} \qquad (6)$$

with $\bar{Q}_s$, $\bar{Q}_p$ and $\bar{Q}_d$ chosen in such a way that the localization of $\bar{S}$ is optimized. We then express eq. (5) in terms of $\bar{S}$ as follows

$$h = (1 + \bar{h}\,\bar{\omega}^{-1})^{-1}\,\bar{h} = \bar{h} - \bar{h}\,\bar{\omega}^{-1}\,\bar{h} + \ldots \qquad (7)$$

with the definitions

$$\bar{h} = \bar{\omega}_- + \bar{\Delta}^{1/2}\,\bar{S}\,\bar{\Delta}^{1/2}$$

$$\bar{\omega} = \omega_- + \frac{\Delta}{\bar{Q}^{-1} - Q^{-1}}$$

$$\bar{\Delta}^{1/2} = [1 + (\bar{Q}^{-1} - Q^{-1})\,\Delta^{-1}\omega_-]\,\Delta^{1/2}$$

and

$$\bar{\omega}_- = [1 + (\bar{Q}^{-1} - Q^{-1})\,\Delta^{-1}\omega_-]\,\omega_-$$

The matrix inversion (6) can only be performed on a lattice and, for the fcc, bcc and sc lattices, it is found[15] that with the following values of $\bar{Q}^{-1}$

0.3485 (s), 0.0530 (p), 0.0107 (d)

the screened structure constants $\bar{S}$ are vanishingly small for the 3rd and higher neighbour distances. Moreover, each two-center integral, e.g. $\bar{S}_{--}$, considered

PHYSICAL REVIEW B VOLUME 44, NUMBER 8 15 AUGUST 1991-II

Electronic-structure calculations for amorphous solids using the recursion method and linear muffin-tin orbitals: Application to $Fe_{80}B_{20}$

H. J. Nowak,* O. K. Andersen, T. Fujiwara,† and O. Jepsen
Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-7000 Stuttgart 80, Federal Republic of Germany

P. Vargas
Universidad de Santiago de Chile, Departamento de Física, P.O. Box 307, Santiago-2, Chile

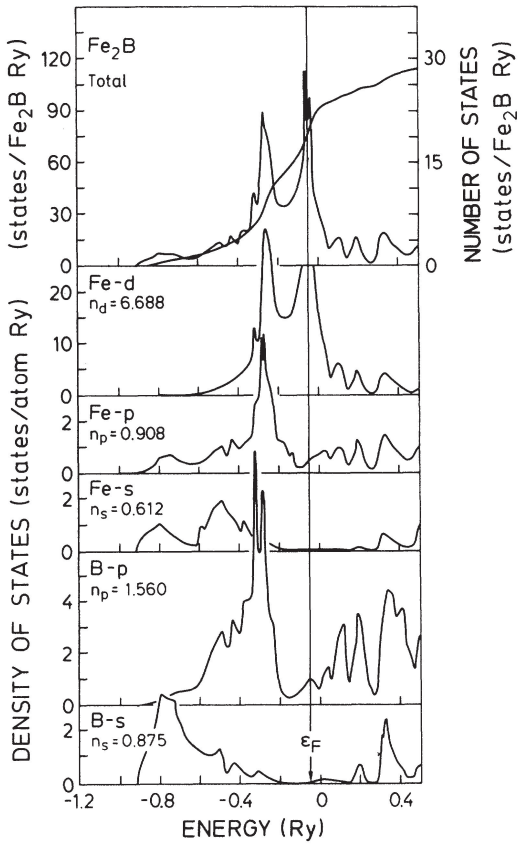
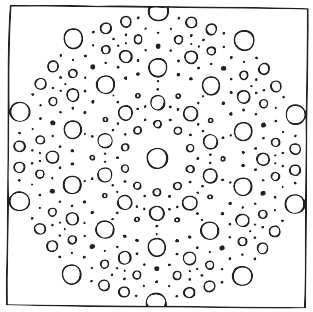
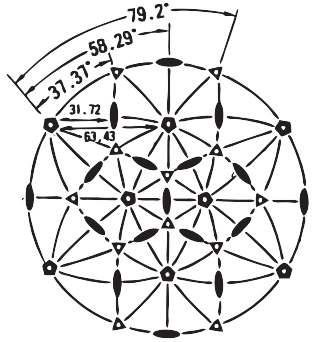


FIG. 4. PDOS and partial occupations for crystalline Fe_2B system obtained by a standard third-order LMTO-ASA band-structure calculation. For boron, only the crystalline *s* and *p* PDOS are shown, the *d* contribution to the occupied part of the DOS is negligible, and the number of *d* electrons is 0.149. In the upper panel, the DOS and the occupation curve per Fe_2B is shown.

‡

（非周期系、実空間計算、大規模系＋大規模行列の対角化）





Journal of the Physical Society of Japan
Vol. 55, No. 5, May, 1986, pp. 1420–1423

LETTERS

PHYSICAL REVIEW B VOLUME 40, NUMBER 2 15 JULY 1989-I

Electronic structure in the Al-Mn alloy crystalline analog of quasicrystals

Takeo Fujiwara
Department of Applied Physics, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan
(Received 23 March 1989)

Electronic structure in crystalline α-($Al_{114}Mn_{24}$) is calculated by the linear muffin-tin orbital–atomic-sphere approximation method with the local-density-functional theory. The density of states consists of a set of spiky peaks. The electronic structure is discussed for quasicrystalline Al-Mn alloy from the viewpoint of the stability and the role of the vacant center of the Mackay icosahedron. The stability is actually owing to the pseudogap of the Mn 3*d* band and the deep *s*,*p*-bonding bands of the Al glue atoms. ‡

Eigenstates in 2-Dimensional Penrose Tiling

Hirokazu TSUNETSUGU, Takeo FUJIWARA, Kazuo UEDA and Tetsuji TOKIHIRO
Department of Applied Physics, University of Tokyo, Tokyo 113 ‡

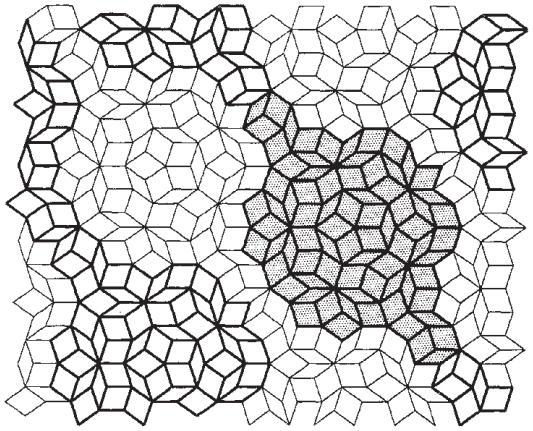


Fig. 1. The (3,2)-periodic Penrose tiling. A shaded region shows a unit cell.

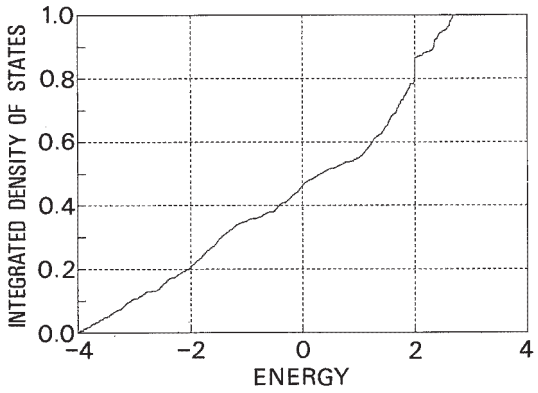


Fig. 2. The integrated density of states of (13,8)-PPT.

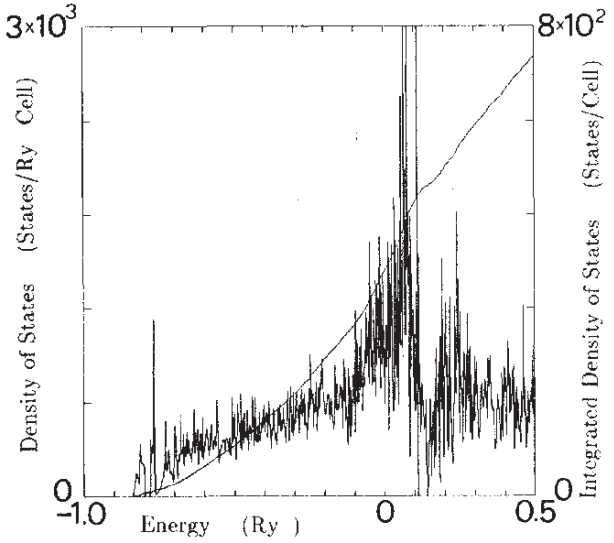


FIG. 1. Total density of states and integrated density of states in a unit cell. The Fermi energy is 0.115 Ry, shown by the vertical line.

Approximant crystal

Pseudo-gap

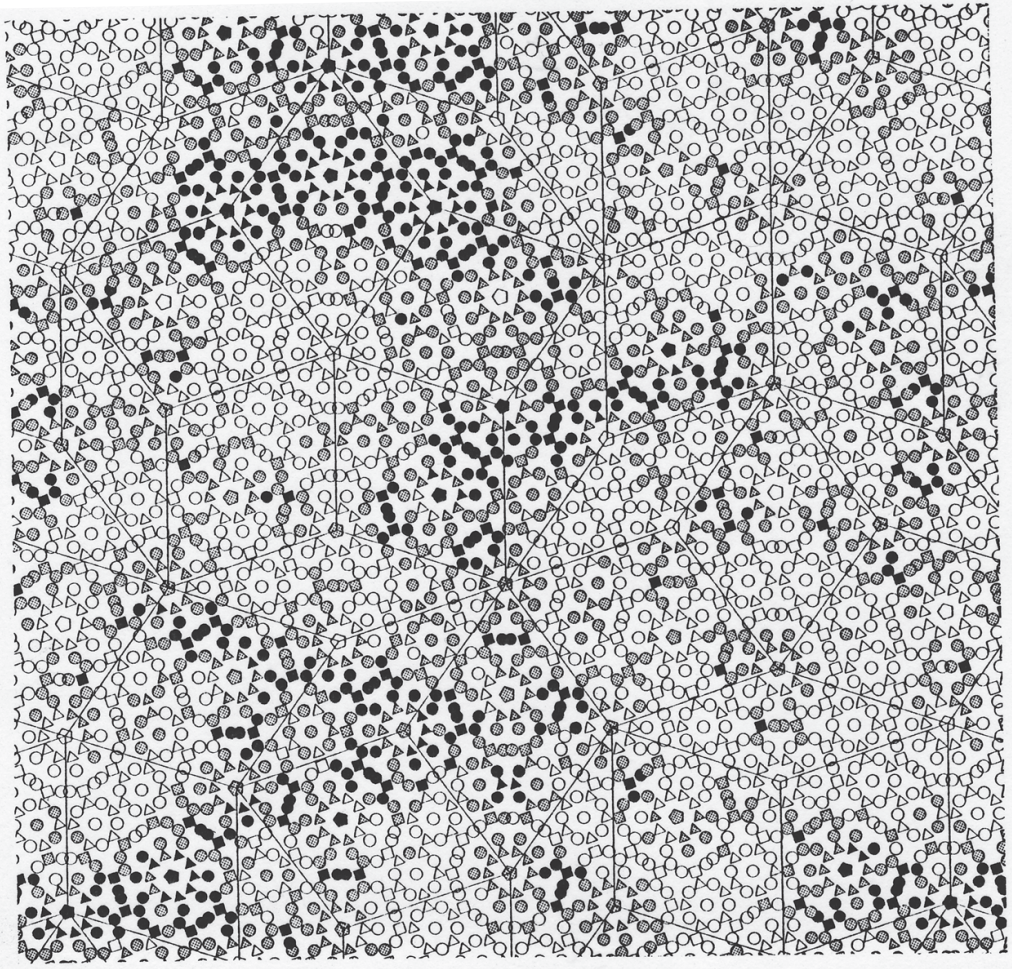


Fig. 3.11. One of exact eigenstates of d-AlCuCo near the Fermi energy in a system of 2728 atoms in a unit cell. The symbols show atomic positions; ○: Al, △: Cu, □: Co. Those atoms represented by the solid symbols are most probable, with the total probability being 60%. Together, the shaded and closed symbols represent those atoms which have a total probability of 90%. The remaining atoms are represented by open symbols.

decagonal AlCuCo

Spatial extent in quasicrystals

Phys. Rev. B53, R2910 (1996) ‡

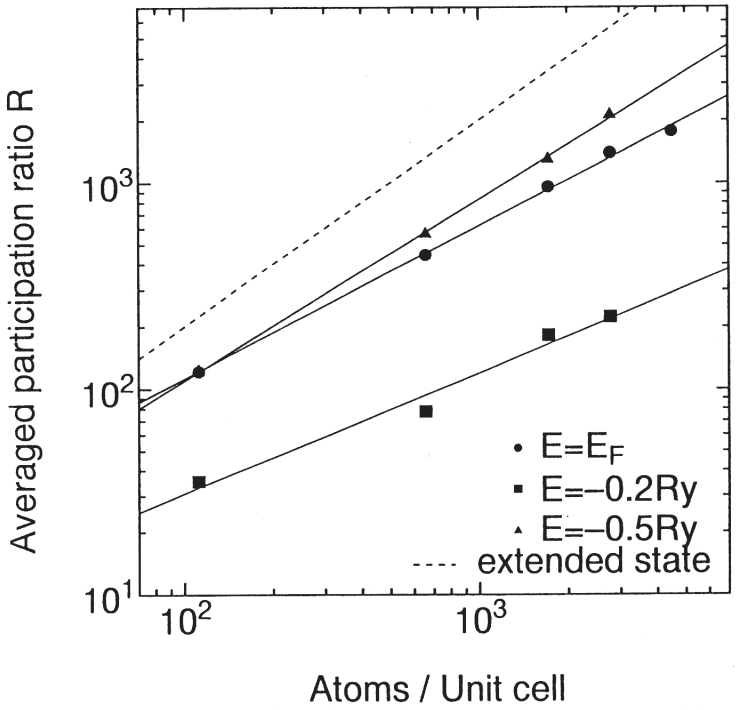


Fig. 3.12. The participation ratio of d-AlCuCo averaged over about 50 eigenstates near Fermi energy E_F (○), 0.2Ry below E_F (□) and 0.5Ry below E_F (△) as a function of the number of atoms N in a unit cell.

(High Tc: Correlated Systems)

JAPANESE JOURNAL OF APPLIED PHYSICS
VOL. 26, No. 5, MAY, 1987, pp. L716-L718

Electronic Structure of High T_c Superconducting Layered Perovskite La-Cu-O and Y-Ba-Cu-O by LMTO Method

Takeo FUJIWARA and Yasuhiro HATSUGAI

Department of Applied Physics, University of Tokyo, Tokyo 113

(Received April 15, 1987; accepted for publication April 25, 1987) ‡

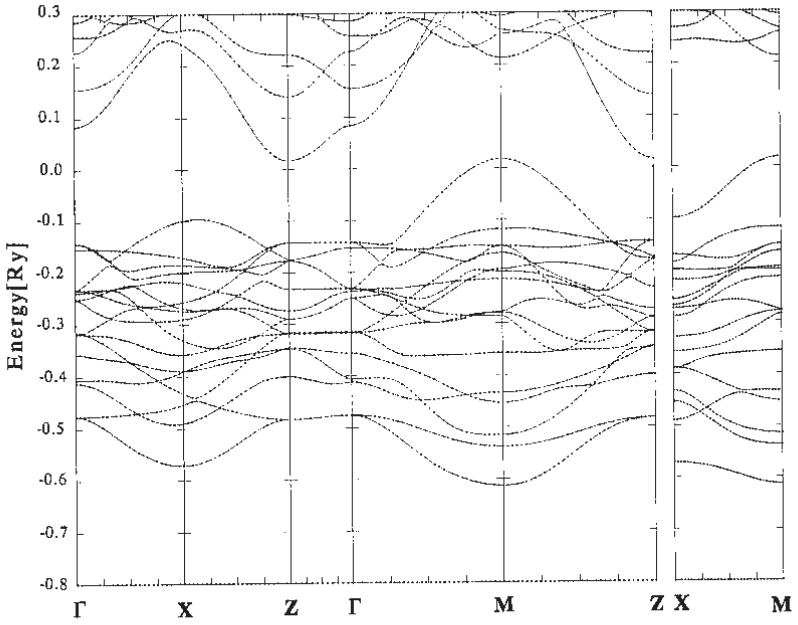
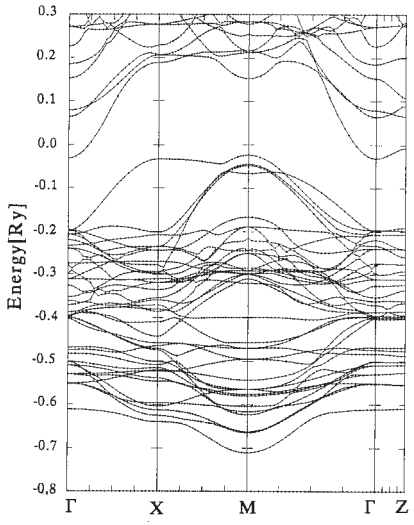
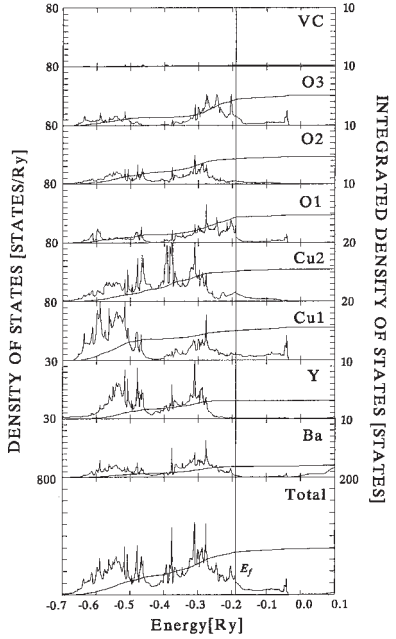


Fig. 1. The band structure of La_2CuO_4.



(a)



(b)

Fig. 2. The band structure (a), DOS and the integrated DOS (b) of $YBa_2Cu_3O_8$. The local ones are for each atom and the total one for one ($YBa_2Cu_3O_8$) unit.

VOLUME 55, NUMBER 22 PHYSICAL REVIEW LETTERS 25 NOVEMBER 1985

Unified Approach for Molecular Dynamics and Density-Functional Theory

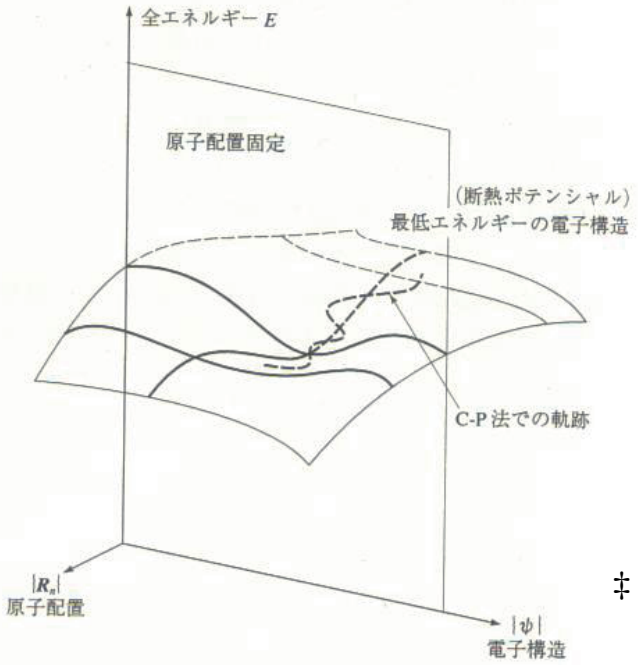
R. Car
International School for Advanced Studies, Trieste, Italy

and

M. Parrinello
Dipartimento di Fisica Teorica, Università di Trieste, Trieste, Italy, and International School for Advanced Studies, Trieste, Italy

(Received 5 August 1985)

‡



‡

$$\mathcal{L} = \sum_n \frac{1}{2} M_n |\dot{\mathbf{R}}_n|^2 + \sum_{j\sigma} f_{j\sigma} \int d\mathbf{r} \mu_e |\dot{\psi}_{j\sigma}(\mathbf{r})|^2$$

$$- E_{DFT}[\{\mathbf{R}_n\}, \{\psi_{j\sigma}\}, \{f_{j\sigma}\}] + \sum_{jk\sigma} \Lambda_{jk:\sigma} f_{j\sigma} f_{k\sigma} \int d\mathbf{r} \psi^*_{j\sigma}(\mathbf{r}) \psi_{k\sigma}(\mathbf{r})$$

$$M_n \ddot{\mathbf{R}}_n = -\nabla_{\mathbf{R}_n} E_{DFT}$$

$$\mu_e \ddot{\psi}_{j\sigma}(\mathbf{r}) = -\frac{\delta E_{DFT}}{\delta \psi^*_{j\sigma}(\mathbf{r})} + \sum_k \Lambda_{jk:\sigma} f_{k\sigma} \psi_{k\sigma}(\mathbf{r}).$$

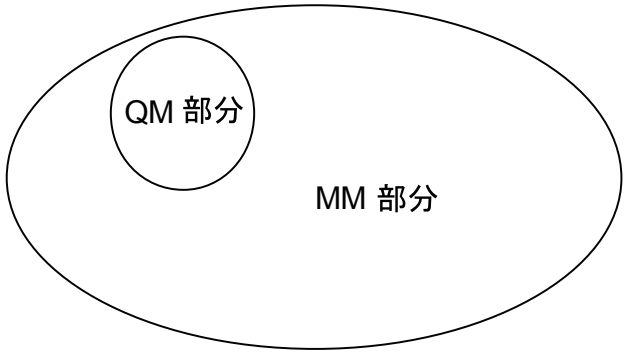
Bio 系の量子力学計算における最近の進歩

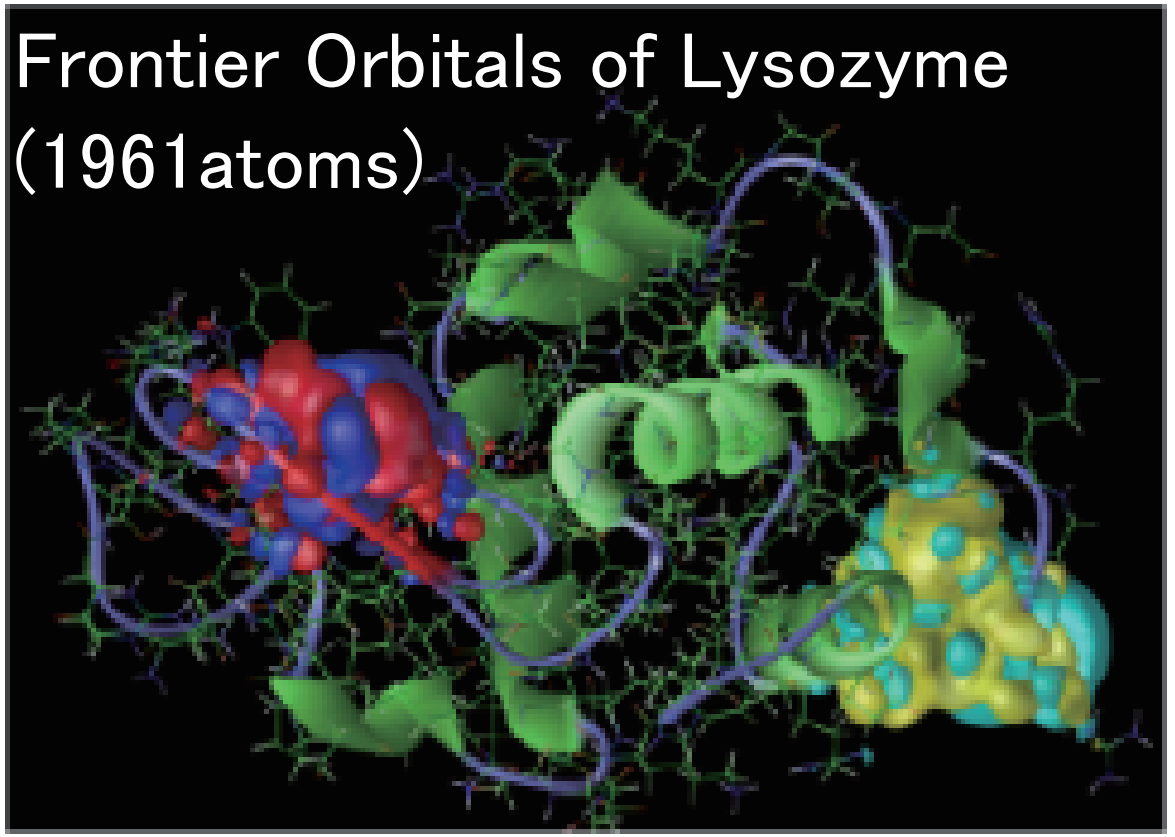
(1)Fragment MO 法…量子論

K.Kitaura et al, Chem Phys. Lett.,336,163(2001)

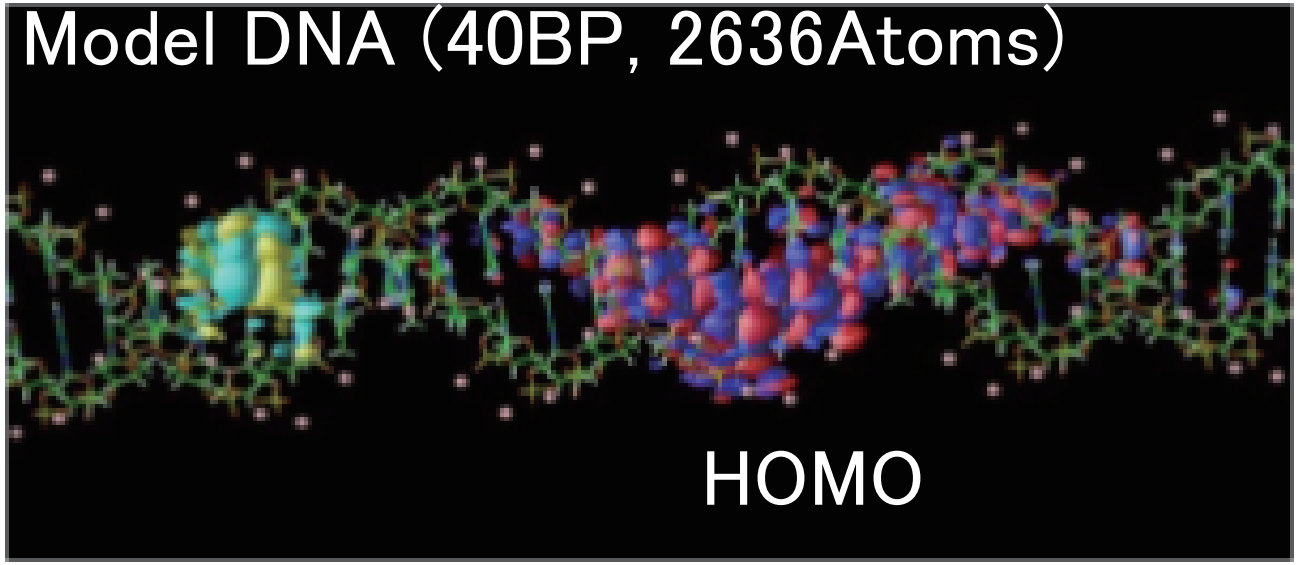
(2) 量子・古典融合法

例：ONIOM 法 (M.Svensson, S.Humbel, R.D.J.Froese, T.Matsubara,S.Sieber,K.Morokuma,J.Phys.Chem.100, 19375(1996)





‡



‡

問題点

1 点計算

最適構造

密度汎関数理論（基底状態）

単一スレーター行列式（SD）

⇔ 揺らぎ

Linear Method （Muffin-Tin 軌道）

実空間表示 ⇔ Bloch の定理

NMTO, EMTO

大規模系 （Order N method）

励起状態

強相関系 （CI, 相互作用）

大規模線型方程式の解法

空間的揺らぎ GW 近似

時間的揺らぎ

動的平均場近似

（DMFT, LDA+DMFT）

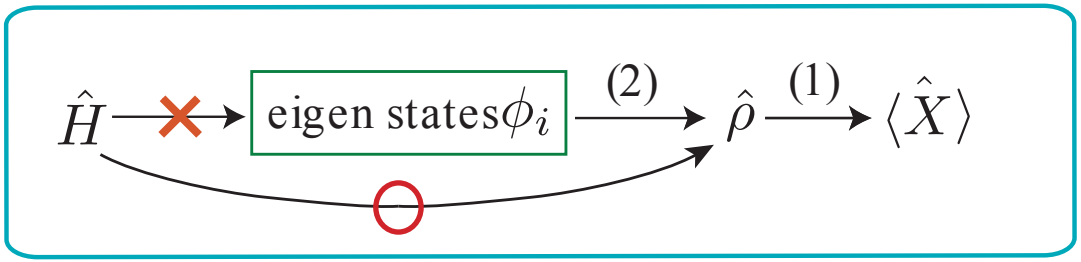
空間・時間揺らぎ

大規模系

アモルファス	ハミルトニアン：実空間形式 大規模計算　（短距離秩序）	LMTO-Recursion 法 tb-LMTO 法
準結晶	ハミルトニアン：実空間形式 大規模計算　（長距離秩序⇔位相）	LMTO- 直接対角化 Forced Oscillator
ナノスケールシステム	ハミルトニアン 大規模計算 長時間プロセス（長時間 MD）	Wannier 表示 Krylov 部分空間法 　直接対角化 　シフト COCG

Large-scale electronic-structure calculations

Witout calculation of extended eigenstates.



Not necessary all of elements of Density Matrix

Calculating a physical quantity $\langle X \rangle$

$$\langle \hat{X} \rangle = \sum_{i}^{\text{occ.}} \langle \phi_i | \hat{X} | \phi_i \rangle = \mathrm{Tr}[\hat{\rho}\hat{\mathrm{X}}] \qquad (1)$$

$$\hat{\rho} \equiv \sum_{i}^{\text{occ}} |\phi_i\rangle\langle\phi_i| \qquad (2)$$

: (one-body) density matrix

Wannier representation.
Hoshi and Fujiwara
J. Phys. Soc. Jpn **69**, 3773 (2000)

Order-N
Hoshi and Fujiwara
J. Phys. Soc. Jpn **72**, 2880 (2003)

Krylov (Subspace Diagonalization)
Takayama, Hoshi and Fujiwara
J. Phys. Soc. Jpn **73**, 1519 (2004)

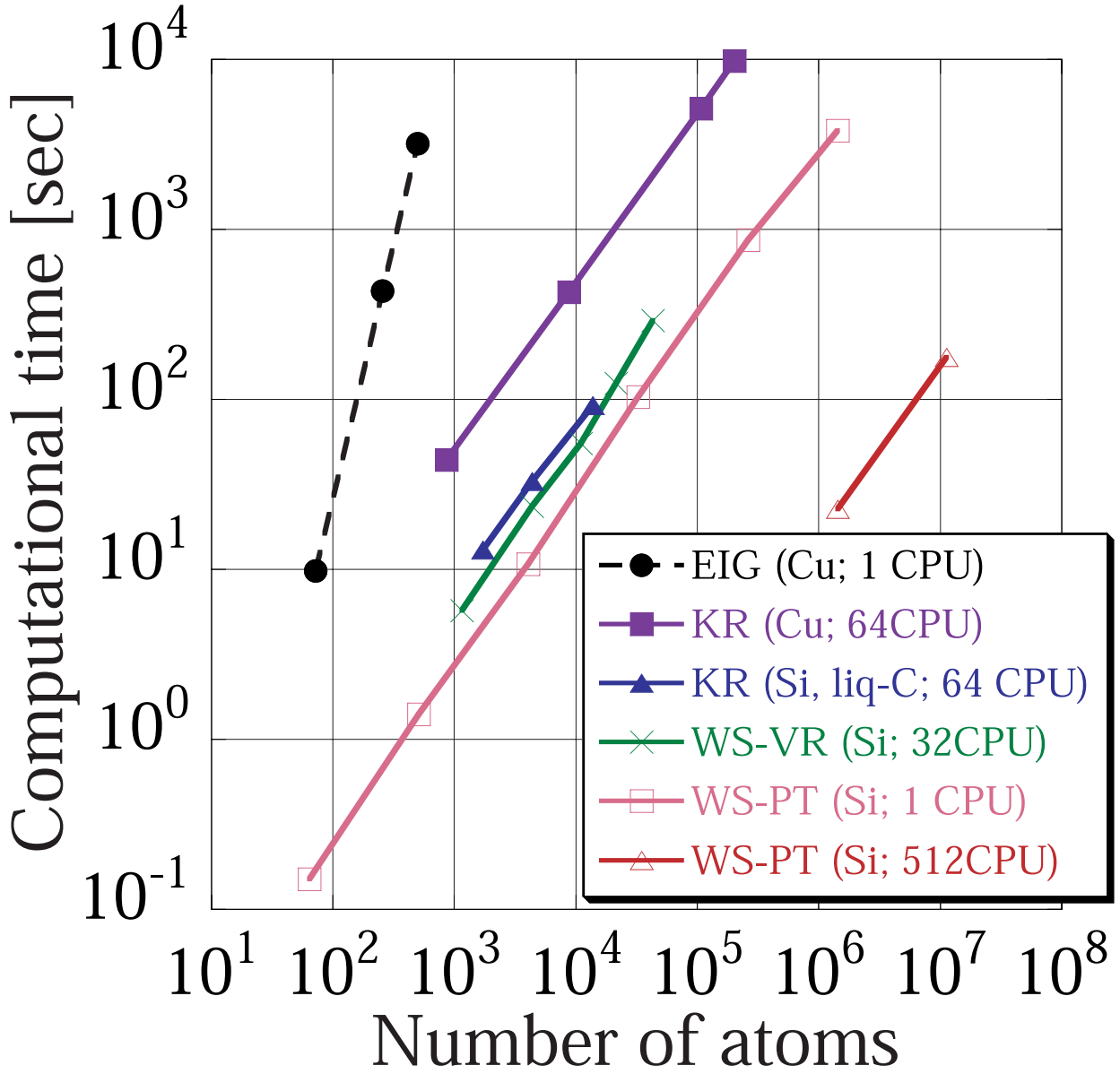
Krylov (Shifted COCG)
Takayama, Hoshi and Fujiwara
Phys. Rev. B73, 165108 (2006)

Large-scale Electronic Structure Calculation

10^7 atoms !!
~$(70\ \mathrm{nm})^3$ system !!

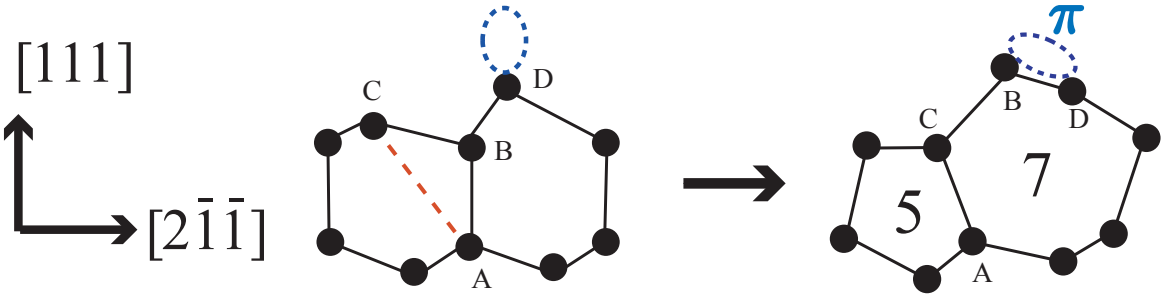
Density Matrix Formalism

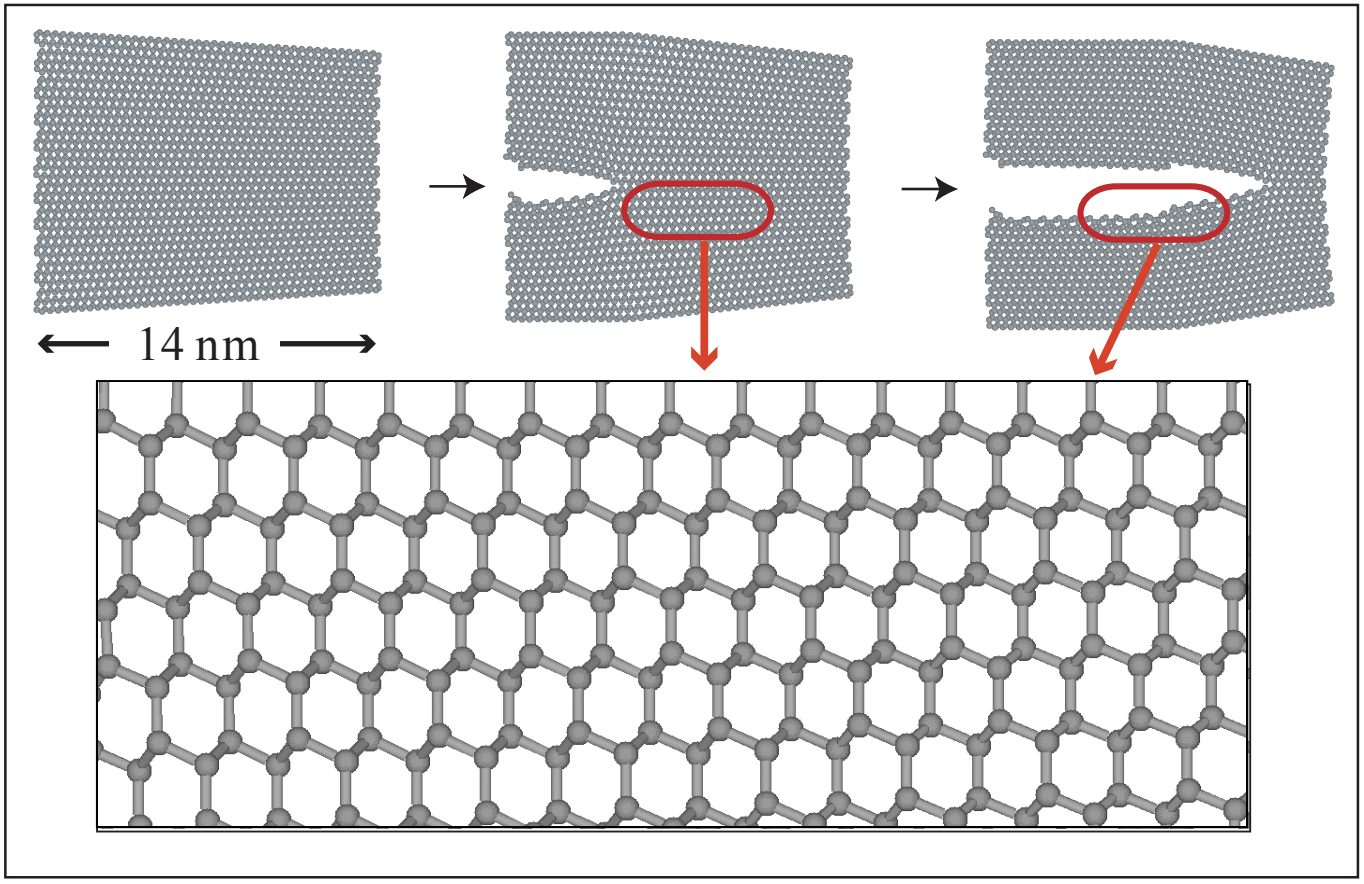
Wannier state representation
Krylov subspace diagonalizatiopn
shifted COCG method
Hybrid method and parallelization



Application : Si(111)-(2x1) cleavage simulation

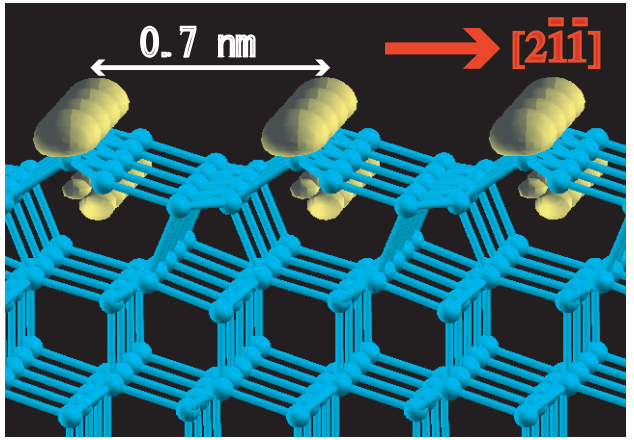
→ π-bonded (Pandey) structure with tilting
Steps are formed in large (10-nm-scale) samples





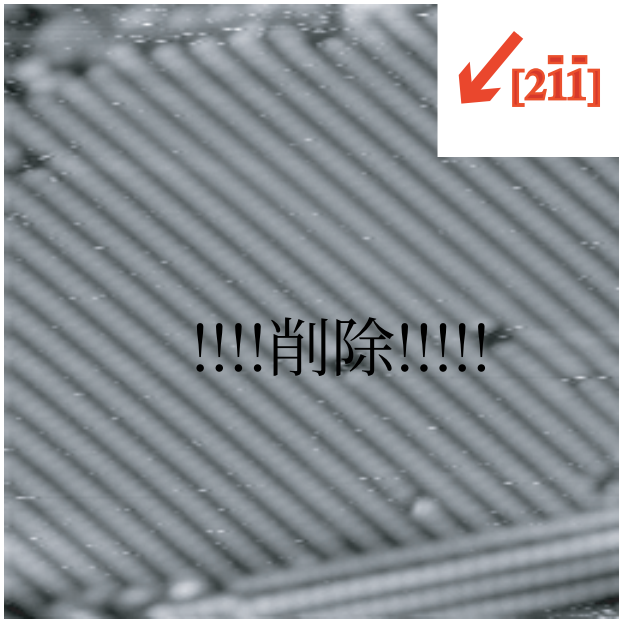
Hoshi, Iguchi and Fujiwara
Phys.Rev. B72, 075323 (2005)

Surface (π-bonding) state



‡

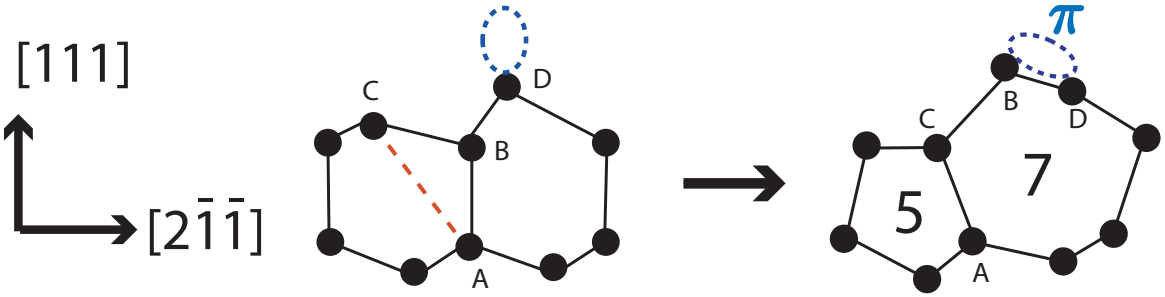
Example of STM experiment

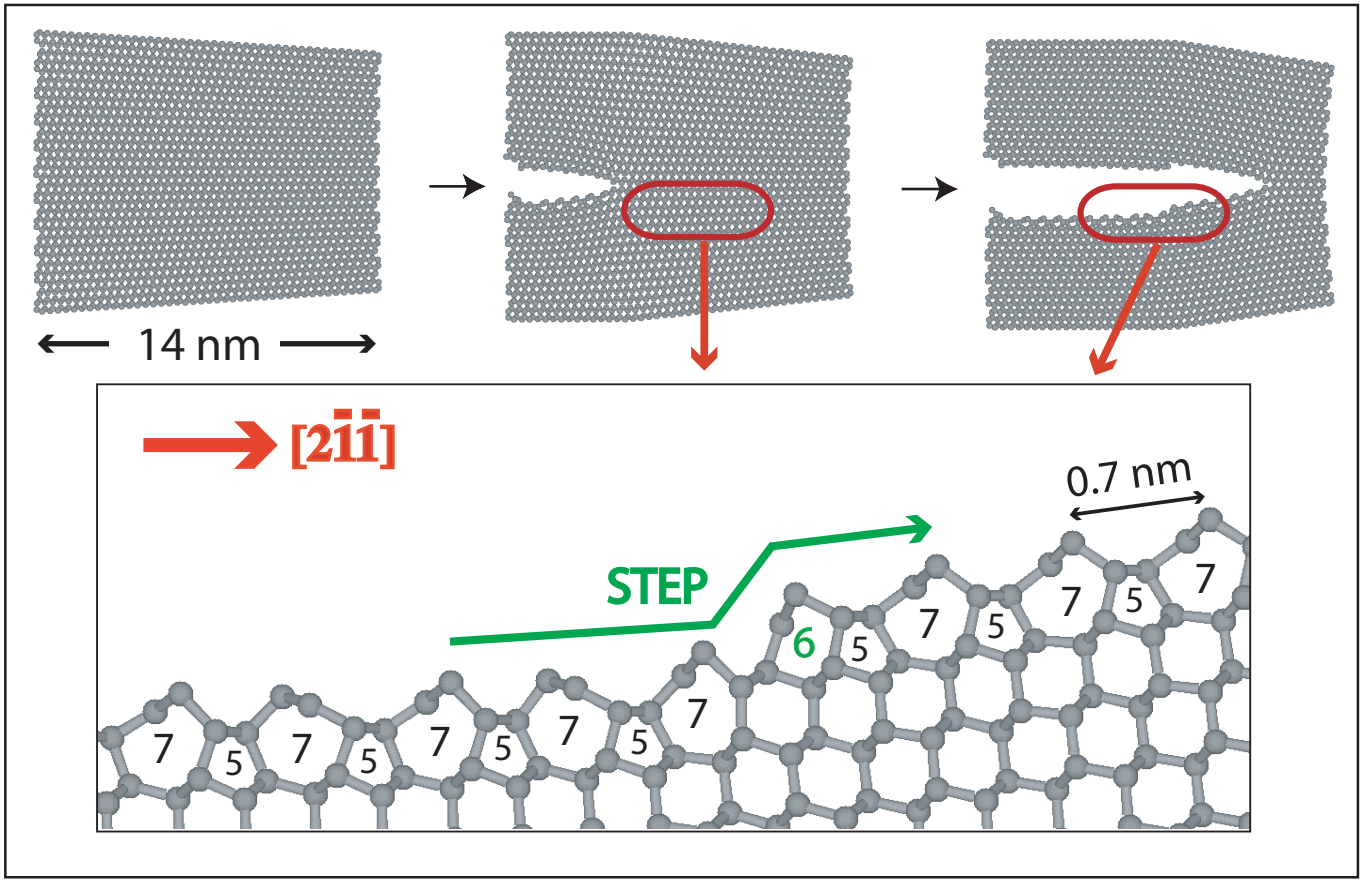


Mera, *et al.*, Ultramicroscopy, (1992)

Application : Si(111)-(2x1) cleavage simulation

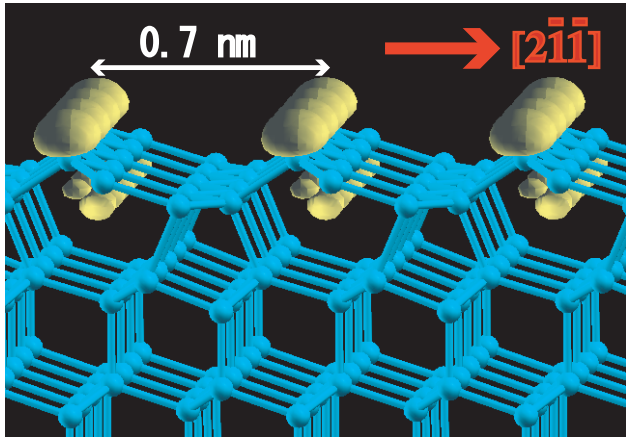
→ π-bonded (Pandey) structure with tilting
Steps are formed in large (10-nm-scale) samples





Hoshi, Iguchi and Fujiwara
Phys.Rev. B72, 075323 (2005)

Surface (π-bonding) state



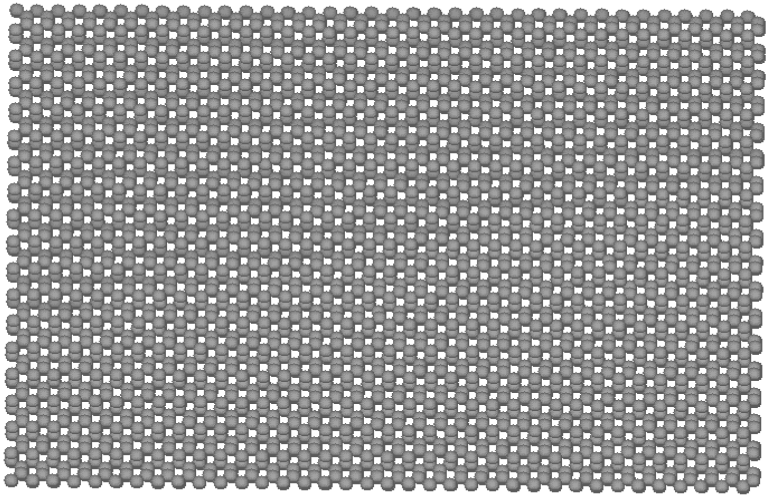
‡

Example of STM experiment

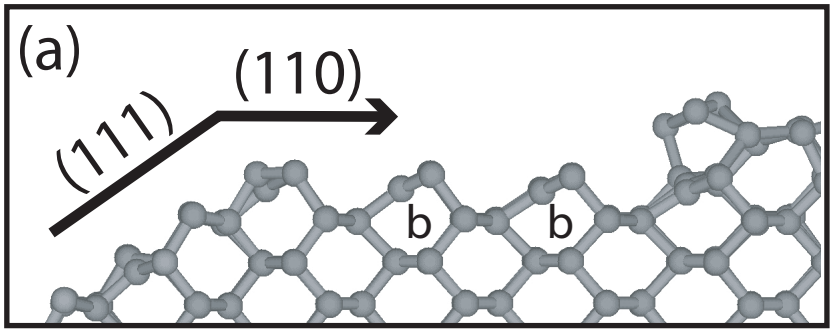


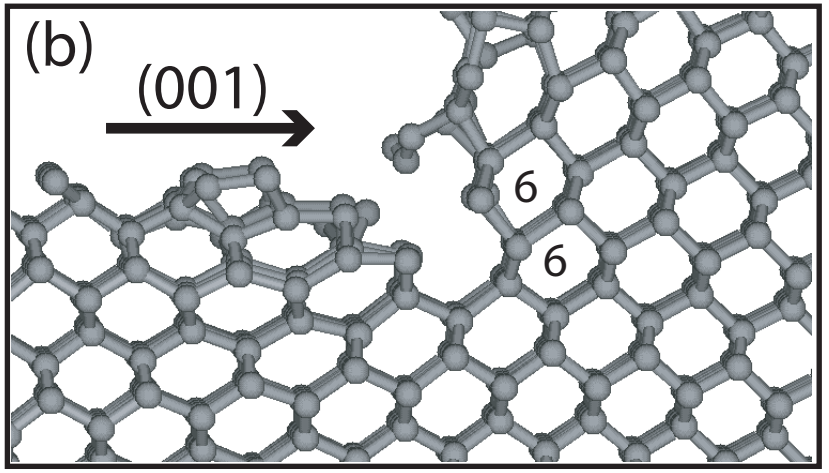
Mera, et al., Ultramicroscopy, (1992)

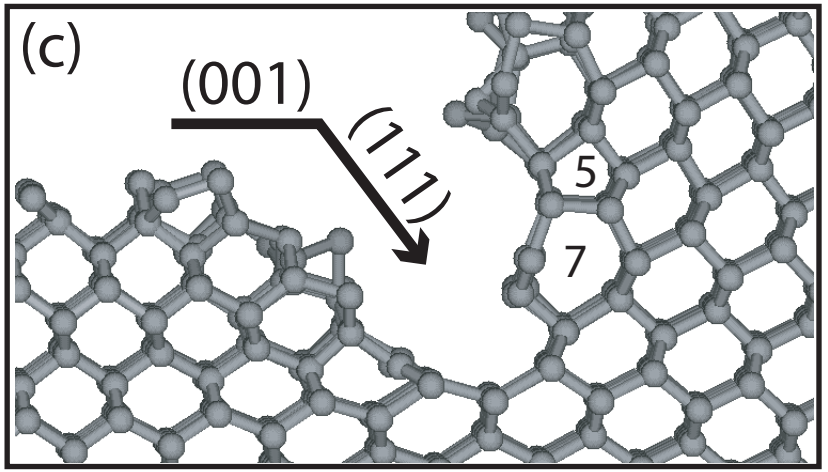
Bending of cleavage path into favorite planes



Hoshi, Iguchi and Fujiwara
Phys.Rev. B72, 075323 (2005)

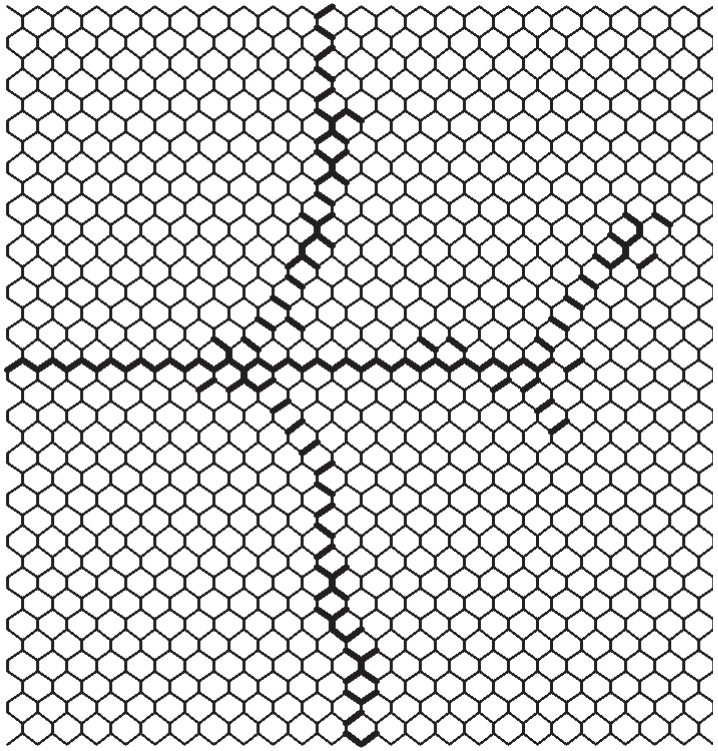


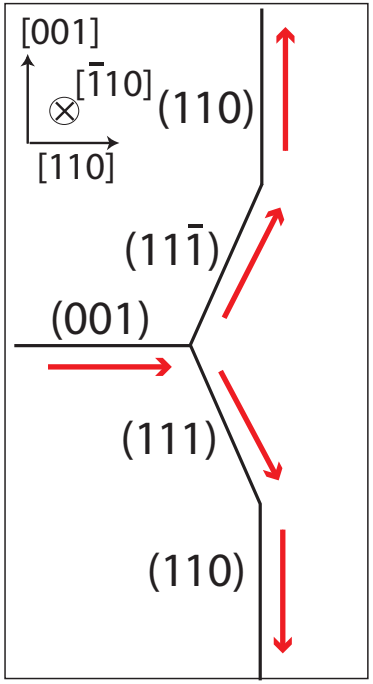


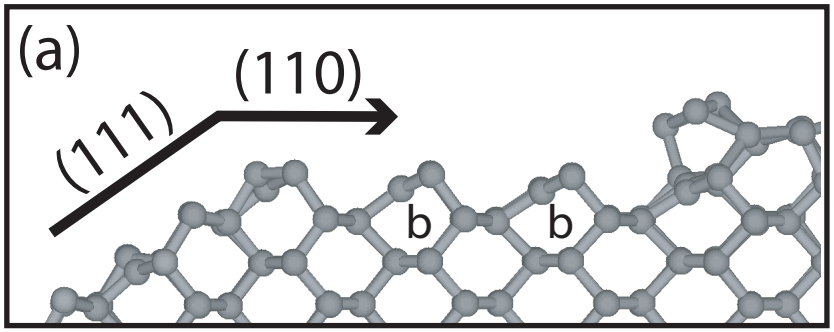


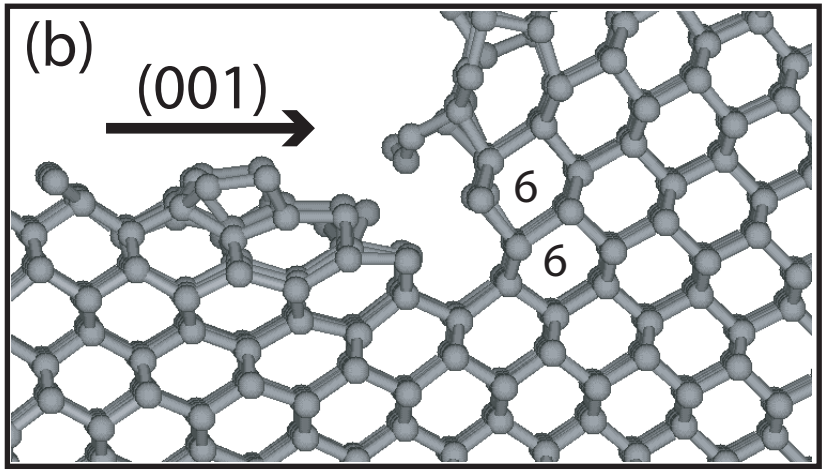
Bending of cleavage path into favorite planes

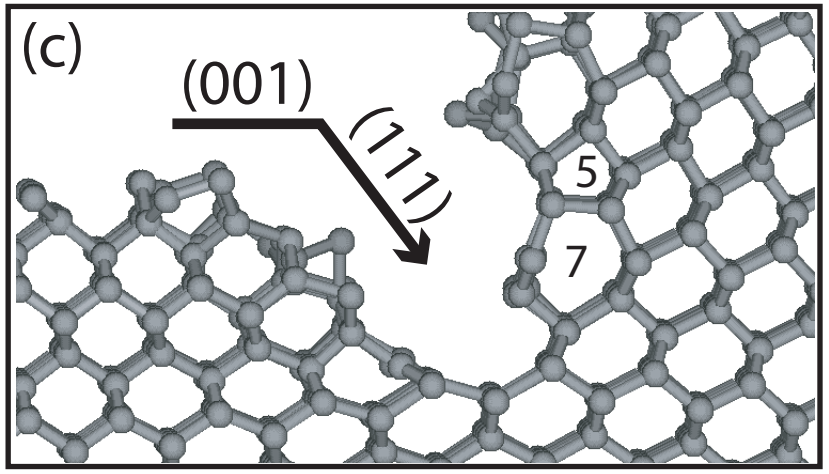
Hoshi, Iguchi and Fujiwara
Phys.Rev. B72, 075323 (2005)









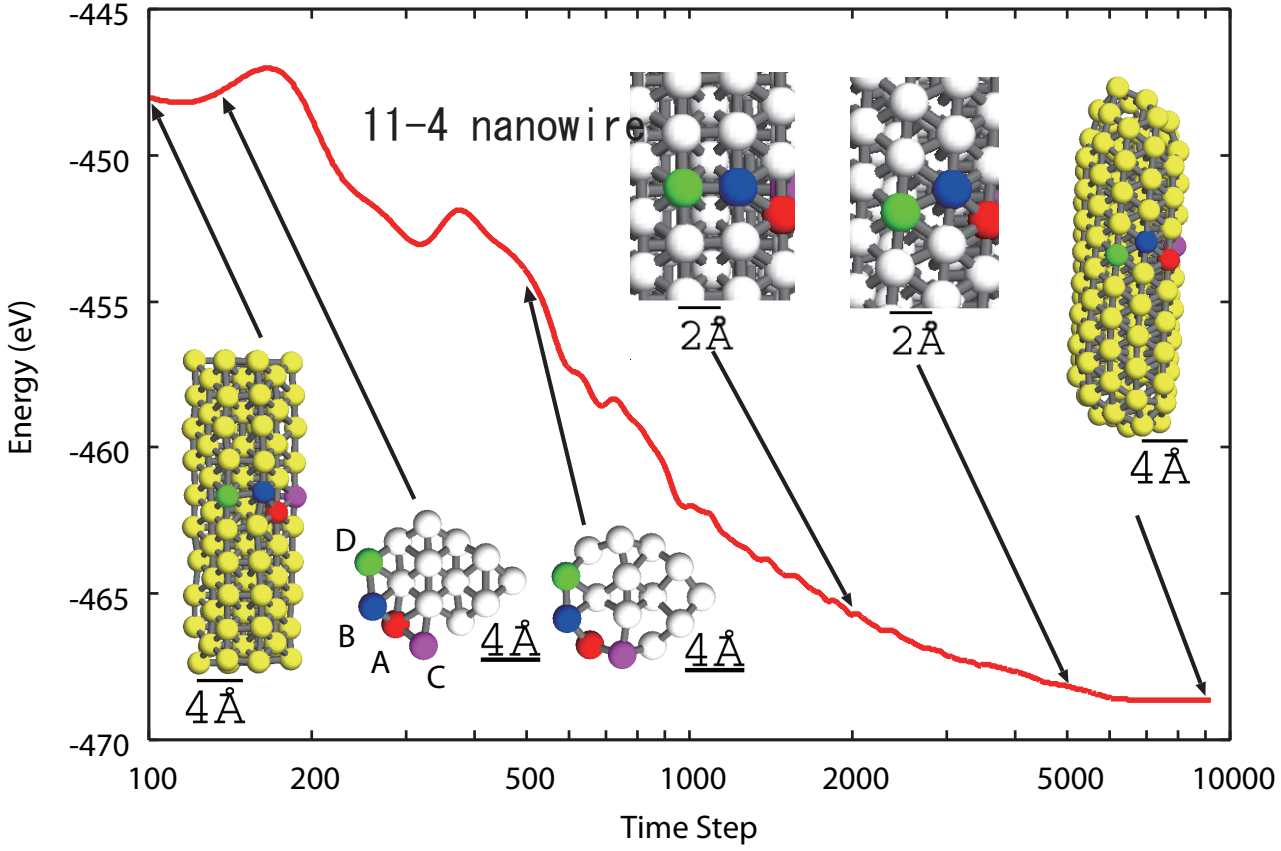


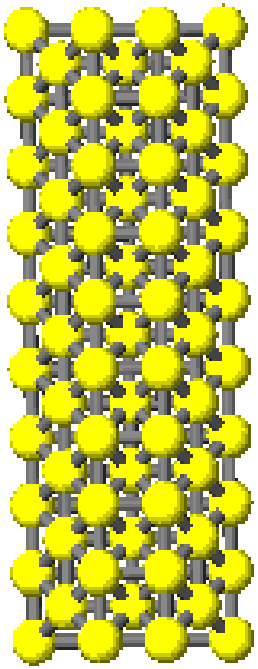
Gold helical multishell nanowires

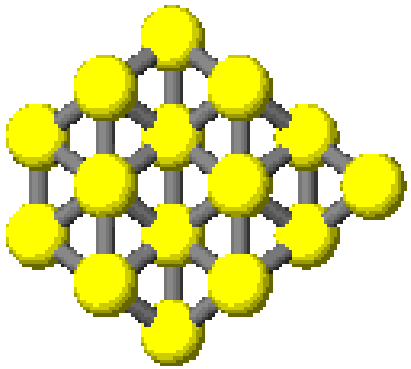
Magic number, Multi-shell structure, Helicity

Iguchi, Hoshi and Fujiwara (2007) ‡

Energy and structure change

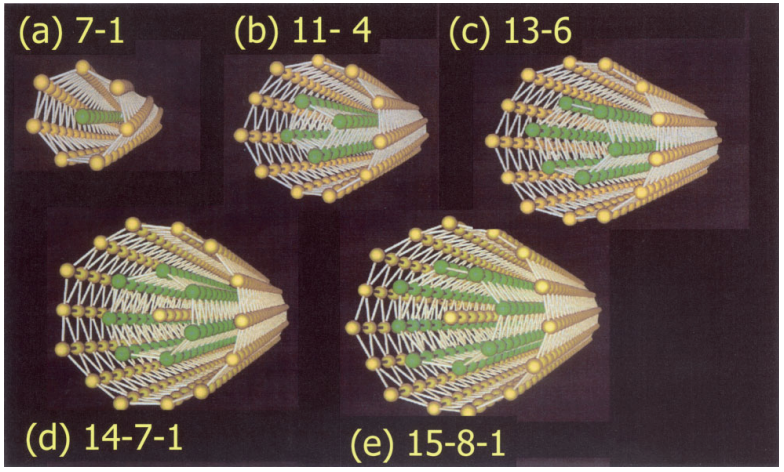




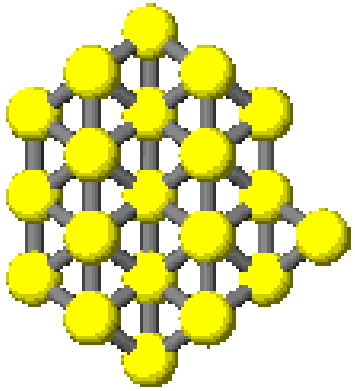


13-6-1

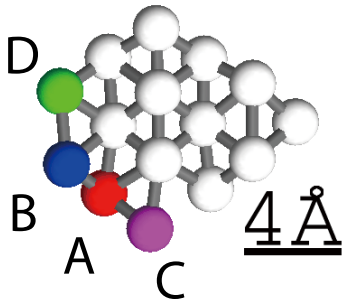
Y.Kondo and K.Takayanagi, Science **289**, 606 (2000)



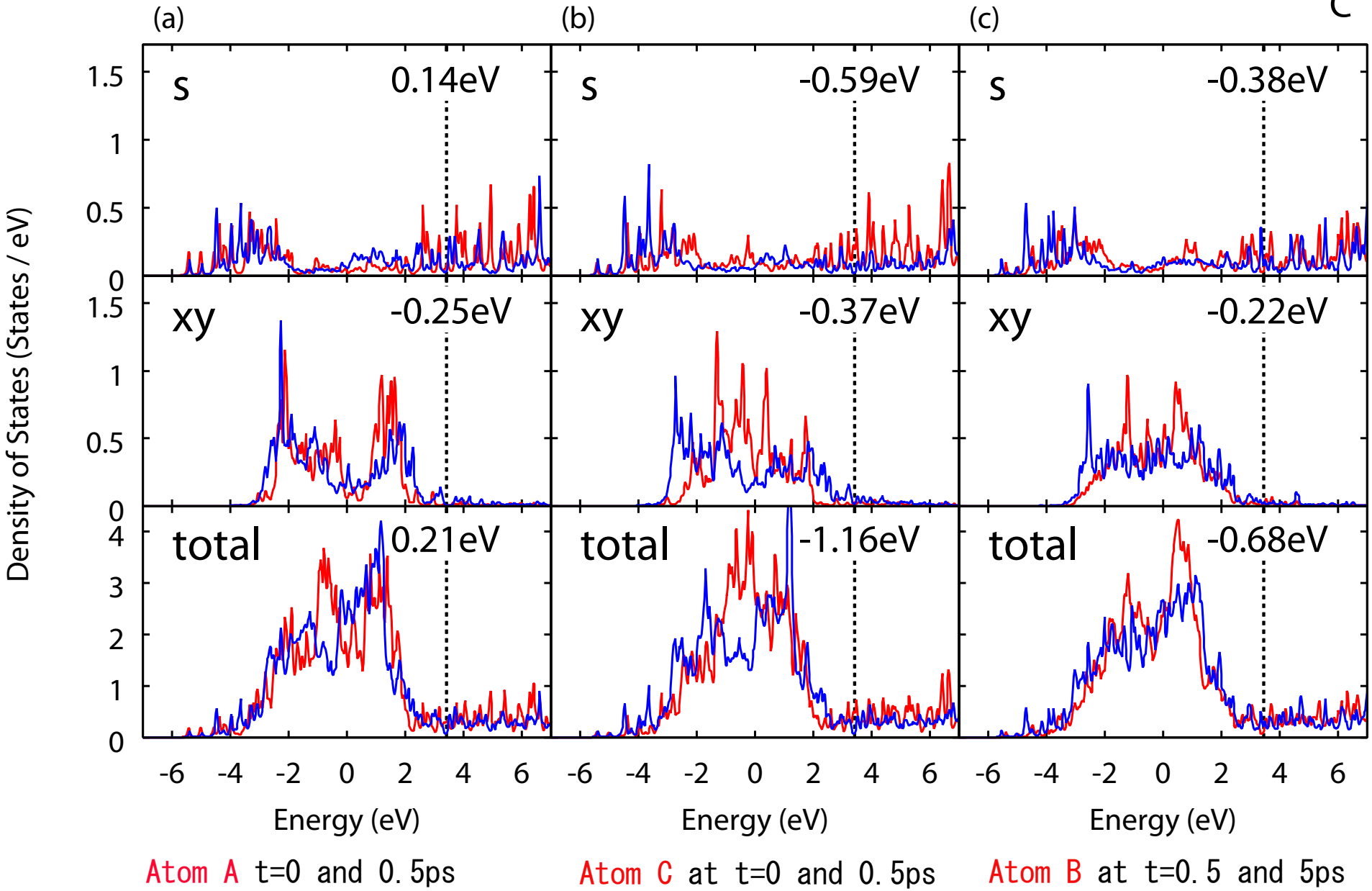
‡



Gold helical multishell nanowires ‡



Local Density of States (11-4 Au nanowire)



Atom A t=0 and 0.5ps

Atom C at t=0 and 0.5ps

Atom B at t=0.5 and 5ps

Electronic structure calculations for large scale systems

$10^4 \sim 10^7$ atoms　　(10～100 nm)

Tight-binding formulation of the total electronic energy

Generalized Wannier states --- Unitarity freedom of eigen states

(1) Density matrix represented by Wannier states

(2) **Insulators / semiconductors**

Krylov Subspace Method

Subspace diagonalization method

Shifted COCG method

(1) Density matrix in Krylov subspace

(2) **Insulators / semiconductors and metals**

Hybrid scheme by dividing the Hilbert space,　Prallelization

Construction of Universal TB-Hamiltonian

密度汎関数理論（基底状態）

⇓

Linear Method （Muffin-Tin 軌道）

NMTO, EMTO

⇓

大規模系 （Order N method）

単一スレーター行列式（SD）

⇔ 揺らぎ

実空間表示 ⇔ Bloch の定理

↘

励起状態

強相関系 （CI, 相互作用）

大規模線型方程式の解法

Hamiltonian の構成

空間的揺らぎ GW 近似

時間的揺らぎ 動的平均場近似

（DMFT, LDA+DMFT）

空間・時間揺らぎ

ナノスケールシステム

相関の強い系

High-Tc (Cuprate),

遷移金属酸化物　etc, etc

手法	電子相関
LDA, LSDA, GGA	RPA, 空間非一様性
LDA-SIC	自己相互作用に対する補正
L(S)DA+U	on-site U（空間揺らぎ） ⇒ ○ Spin Gap × Coulomb Gap, (Hubbard Gap)
GW 近似	動的遮蔽
U+GW 近似	
DMFT(Dynamical Mean Field Theory)	動的揺らぎ(on-ste)
LDA+DMFT	⇒ Hubbard Gap Coherent peak
量子モンテカルロ法	

Constraint LSDA

$$
\begin{aligned}
E_{\mathrm{LSDA}}(n_\uparrow, n_\downarrow) &= E_0 + n\varepsilon_d^0 + \frac{1}{2}n(n-1)U \\
&\quad -\frac{1}{2}n_\uparrow(n_\uparrow - 1)J - \frac{1}{2}n_\downarrow(n_\downarrow - 1)J \\
\varepsilon_{\mathrm{LSDA,d}\sigma}(n_\uparrow, n_\downarrow) &= \frac{\partial E_{\mathrm{LSDA}}(n_\uparrow, n_\downarrow)}{\partial n_\sigma} \\
&= \varepsilon_d^0 + (n - \frac{1}{2})U - (n_\sigma - \frac{1}{2})J
\end{aligned}
$$

$\Rightarrow$

$$
\begin{aligned}
U &= \varepsilon_{\mathrm{LSDA,d}\uparrow}(\frac{n}{2} + \frac{1}{2}, \frac{n}{2}) - \varepsilon_{\mathrm{LSDA,d}\uparrow}(\frac{n}{2} + \frac{1}{2}, \frac{n}{2} - 1) \\
J &= \varepsilon_{\mathrm{LSDA,d}\downarrow}(\frac{n}{2} + \frac{1}{2}, \frac{n}{2} - \frac{1}{2}) - \varepsilon_{\mathrm{LSDA,d}\uparrow}(\frac{n}{2} + \frac{1}{2}, \frac{n}{2} - \frac{1}{2})
\end{aligned}
$$

LDA-SIC（Self-interaction Correction, 自己相互作用補正）

LDA エネルギー汎関数では、自分自身が作るクーロン相互作用を感じる.

$$E^{\mathrm{LDA-SIC}} = E^{\mathrm{LDA}}[n_\uparrow, n_\downarrow] + \sum_{i\sigma} E^{\mathrm{SIC}}[n_{i\sigma}]$$

$$E^{\mathrm{SIC}}[n_{i\sigma}] = -\Big\{ E_{\mathrm{H}}[n_{i\sigma}] + E^{\mathrm{LDA}}_{\mathrm{xc}}[n_{i\sigma}, 0]$$

LDA+U（クーロン相互作用による電荷揺らぎ）

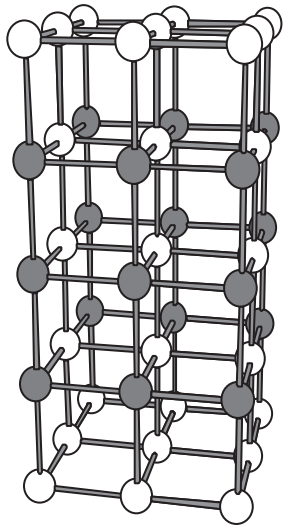
$$n^\sigma_{mm'} = -\frac{1}{\pi}\int^{E_F} dE\ \mathrm{Im}\ G^\sigma_{ilm;ilm'}(E) = \sum_{n\boldsymbol{k}} \langle \phi^\sigma_m | \psi_{n\boldsymbol{k}} \rangle \langle \psi_{n\boldsymbol{k}} | \phi^\sigma_{m'} \rangle$$

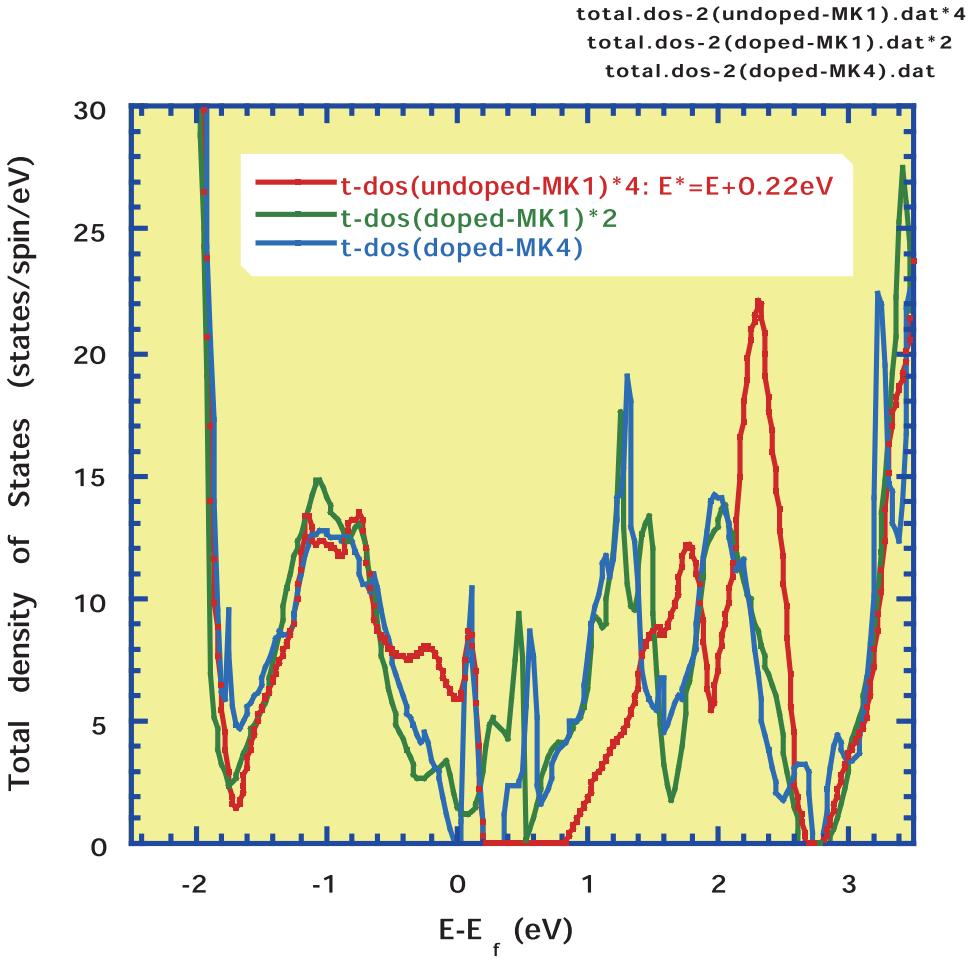
$$\begin{aligned}
E^{LSDA+U}[\{n_\sigma\}, \{n^\sigma_{mm'}\}] &= E^{LSDA}[\{n_\sigma\}] + E^U[\{n^\sigma_{mm'}\}] - E_{dc}[\{n^\sigma_{mm'}\}], \\
E^U[\{n^\sigma_{mm'}\}] &= \frac{1}{2}\sum_{\{m\}\sigma} \Big\{ \langle mm'' | V_{ee} | m'm''' \rangle n^\sigma_{mm'} n^{-\sigma}_{m''m'''} \\
&\quad + \Big(\langle mm'' | V_{ee} | m'm''' \rangle - \langle mm'' | V_{ee} | m'''m' \rangle \Big) n^\sigma_{mm'} n^\sigma_{m''m'''} \Big\}, \\
E_{dc}[\{n^\sigma_{mm'}\}] &= \frac{1}{2} U n(n-1) - \frac{1}{2} J \Big[n_\uparrow(n_\uparrow - 1) + n_\downarrow(n_\downarrow - 1) \Big] .
\end{aligned}$$

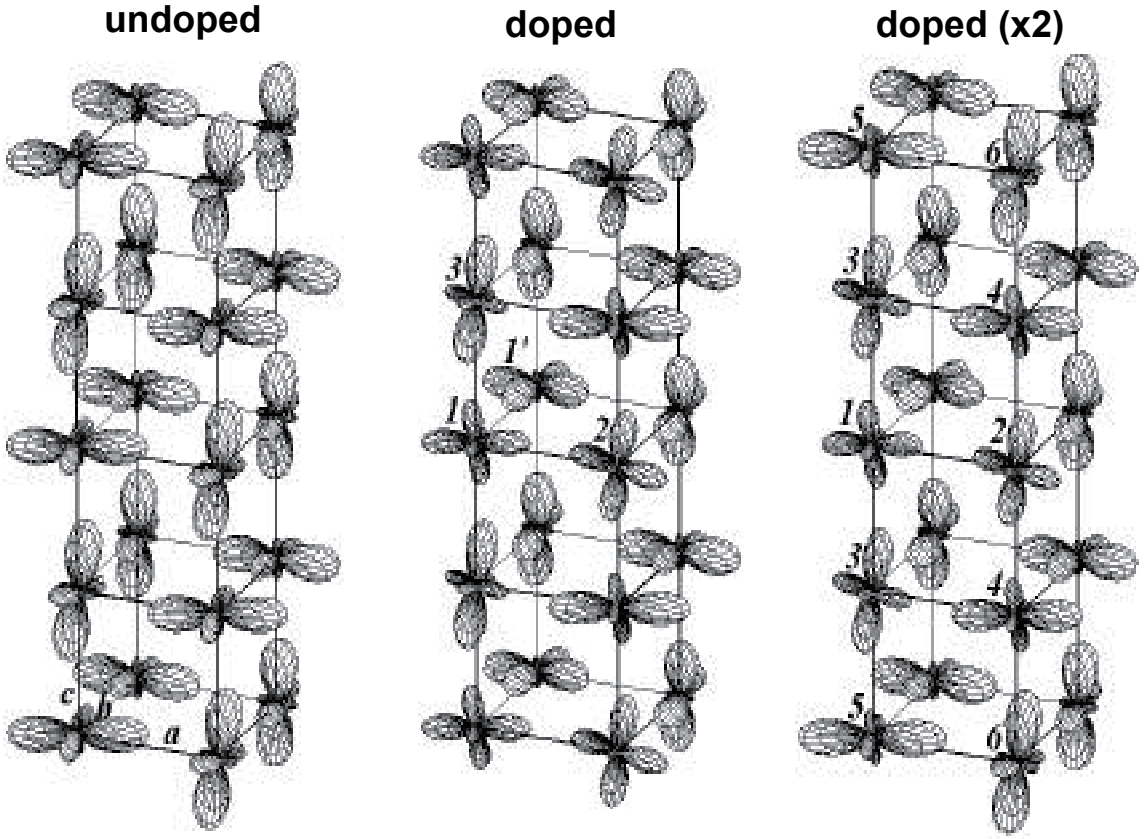
$$\begin{aligned}
V^\sigma_{mm'} &= V^\sigma_{LSDA}\delta_{mm'} + \sum_{m''m'''} \Big\{ \langle mm'' | V_{ee} | m'm''' \rangle n^{-\sigma}_{m''m'''} \\
&\quad + \Big(\langle mm'' | V_{ee} | m'm''' \rangle - \langle mm'' | V_{ee} | m'''m' \rangle \Big) n^\sigma_{m''m'''} \Big\} \\
&\quad + \Big\{ -U(n - \frac{1}{2}) + J(n_\sigma - \frac{1}{2}) \Big\} \delta_{mm'}
\end{aligned}$$

Orbital and charge ordering in $La_{1/2}Sr_{1/2}MnO_3$

Korotin, Fujiwara and Anisimov
PRB **62**, 5696 (2000) ‡

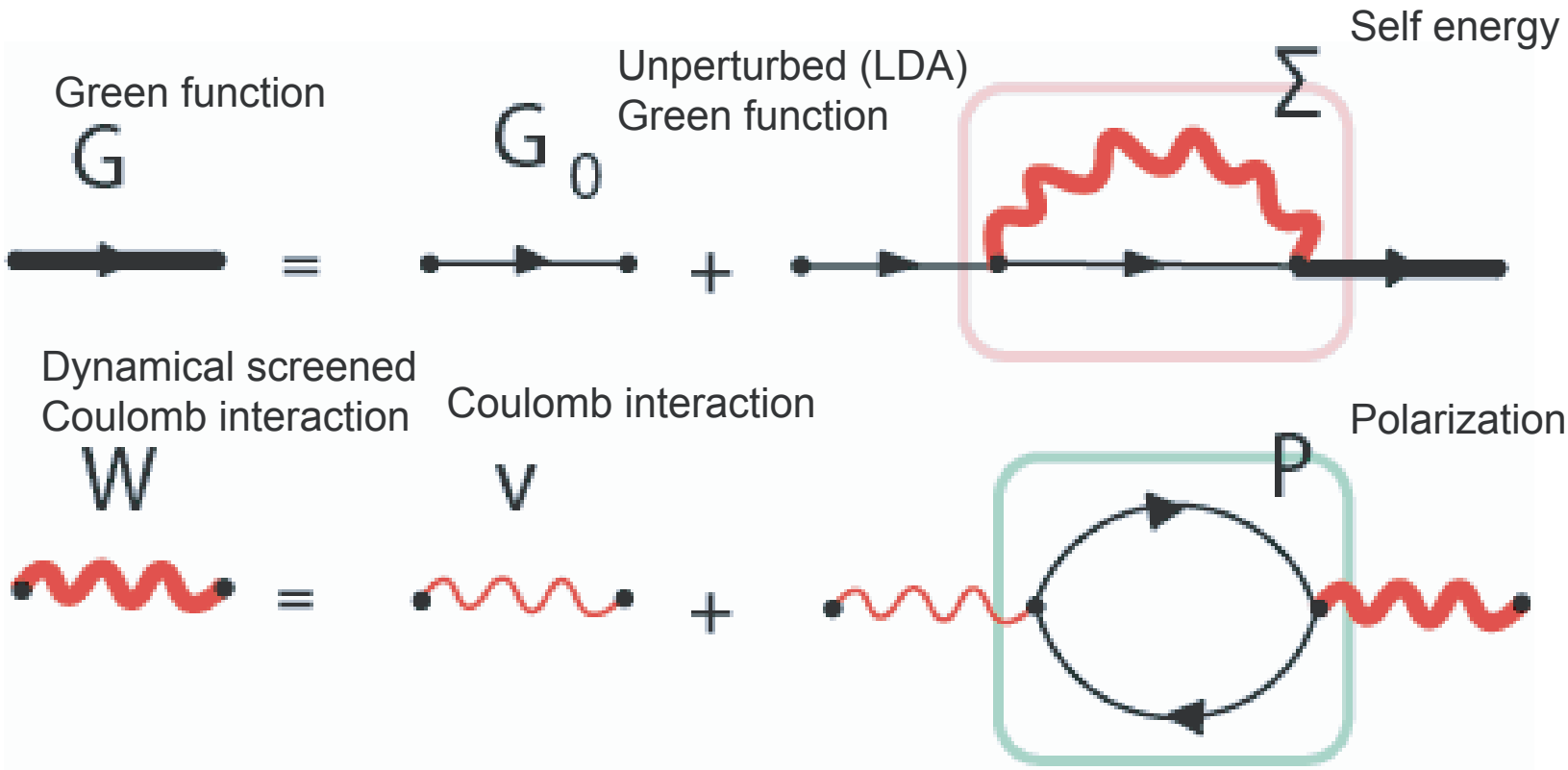






GW-approximation

‡



P : Polarization function of RPA

$$P = -iG_0 G_0$$

$$\Sigma = iG_0 W$$

(L. Hedin, Phys. Rev. A **139**, 796 (1965))

Off-set method, Product-Basis, Parallel Computation etc.

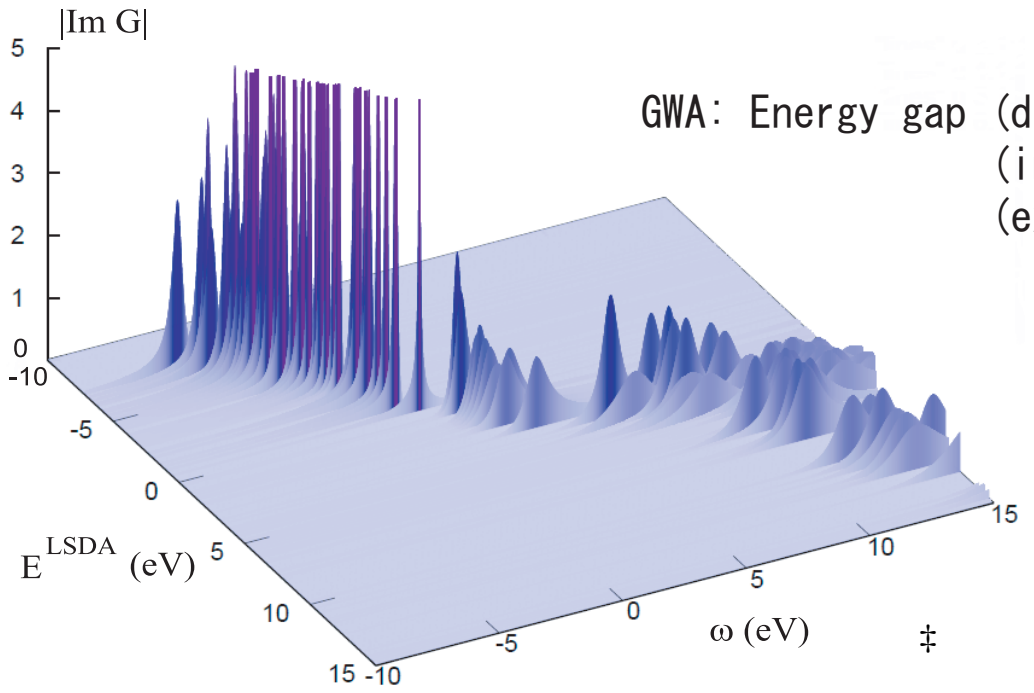
$LaMnO_3$

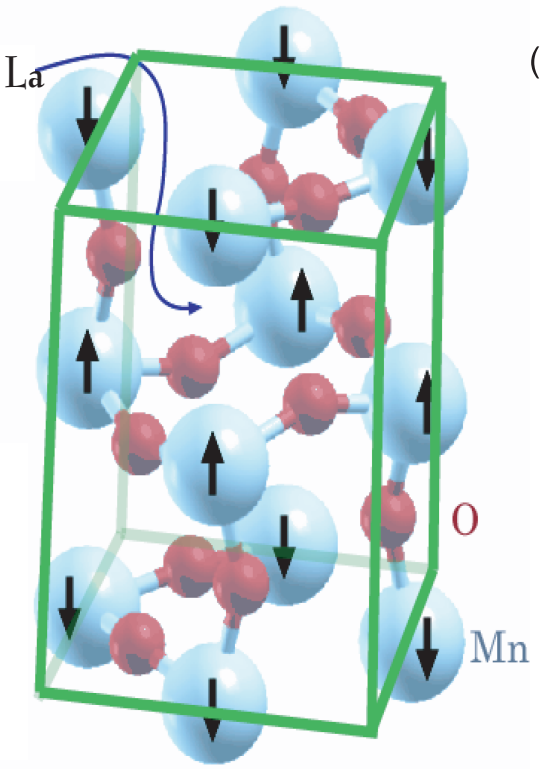
A-type Antiferromagnet

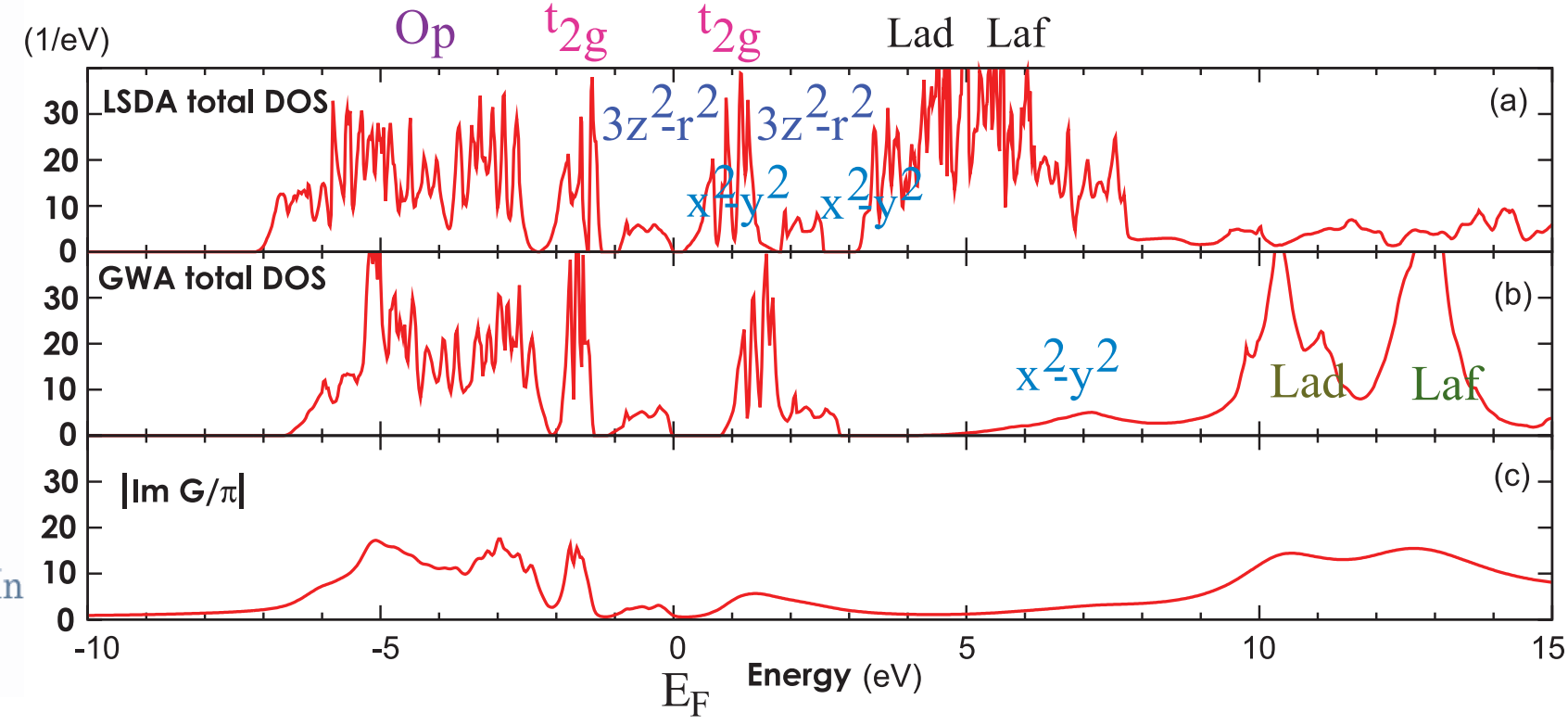
C-type orbital order

GW-approximation

G_0 : LSDA

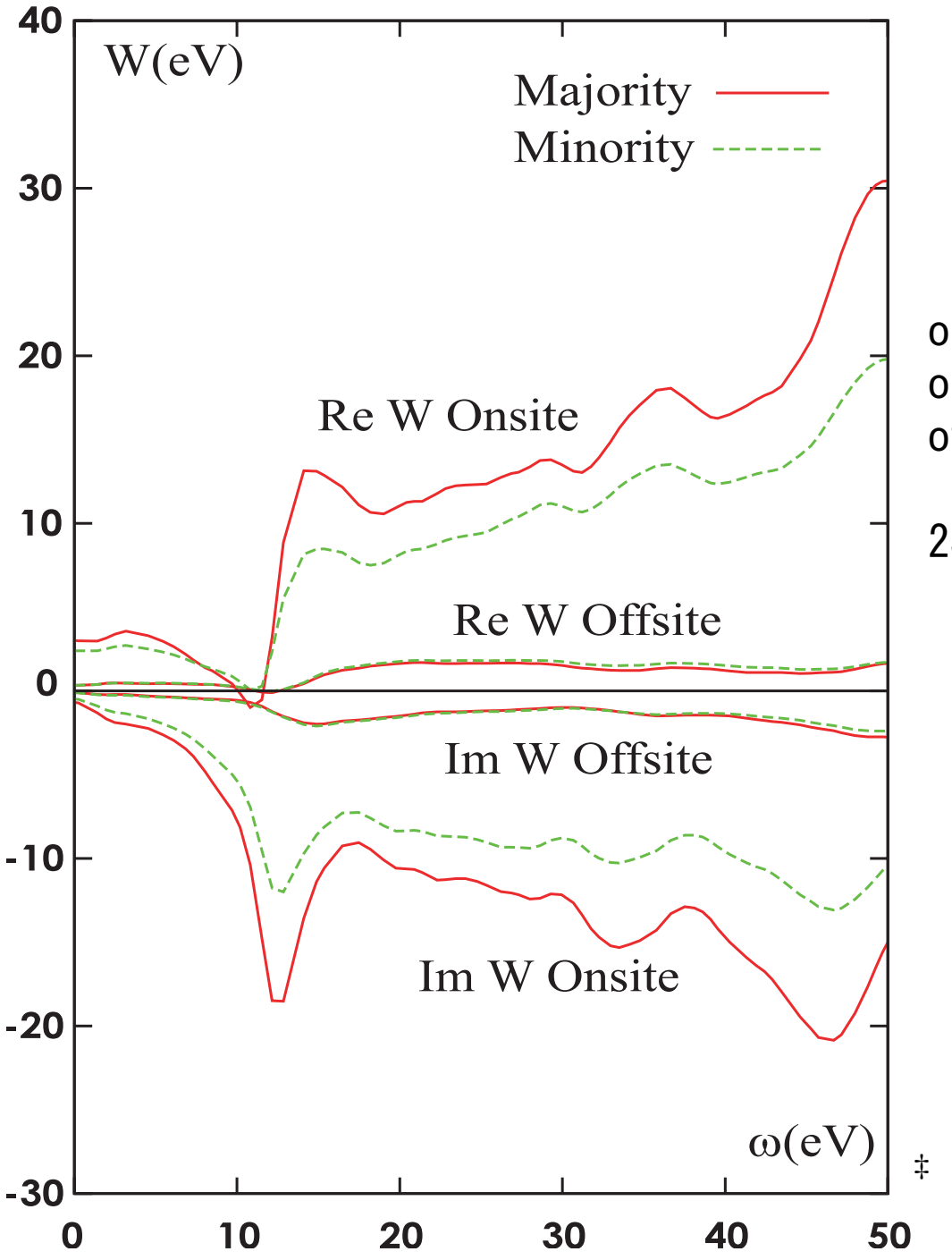






Nohara, Yamasaki, Kobayashi and Fujiwara, Phys. Rev. B **74**, 064417 (2006)

Screened Coulomb interaction *W* [eV] on Mn sites



GW-approximation

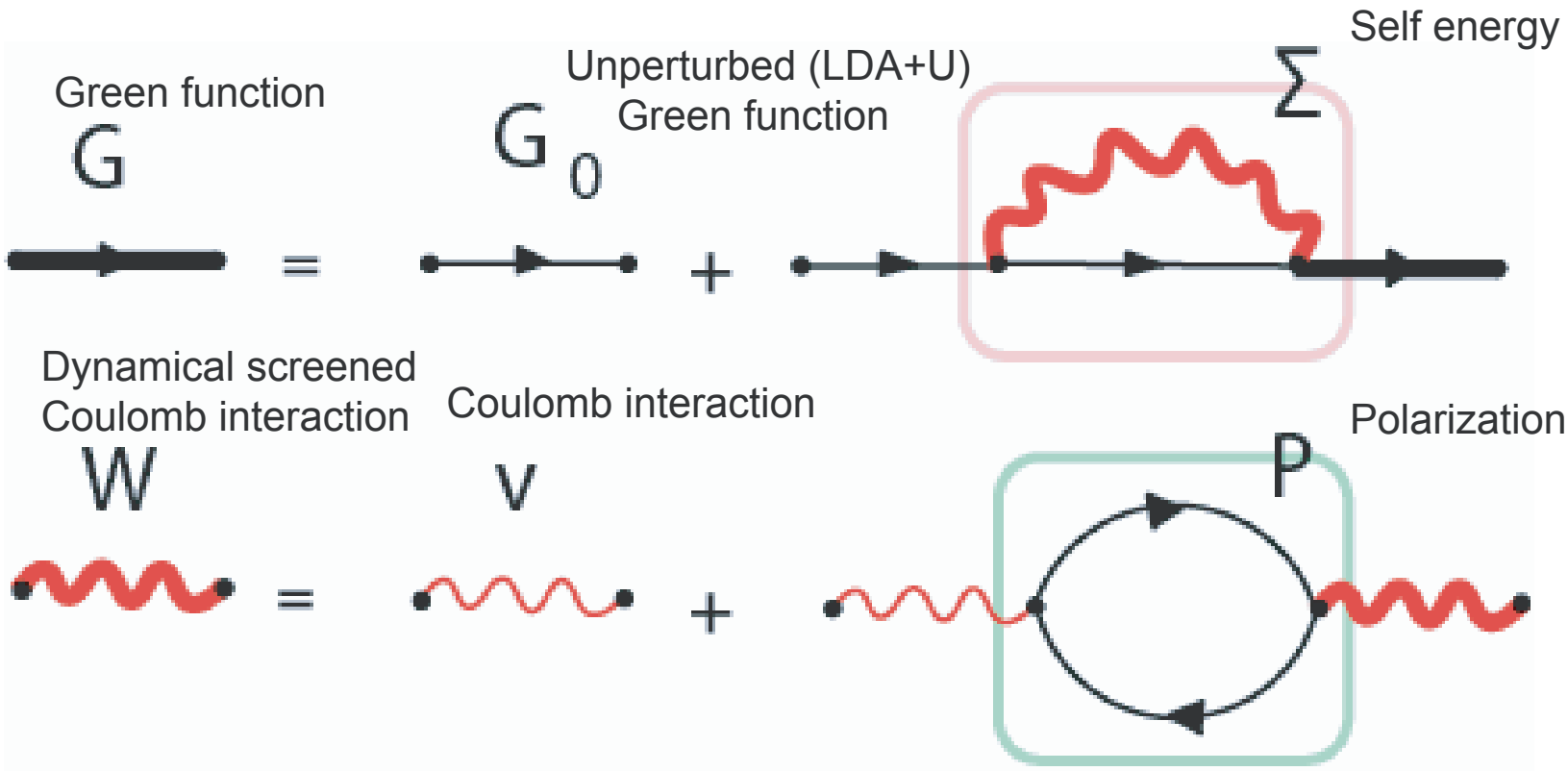
onsite (majority spins):3.00 eV
onsite (minority spins):2.40 eV
offsite(majority and minority spins):0.34 eV

23.4, 17.2, 3.7 eV (high energies)

Phys. Rev. B 74, 064417 (2006)

U+GW-approximation

better $G_0 \Leftarrow$ L(S)DA+U



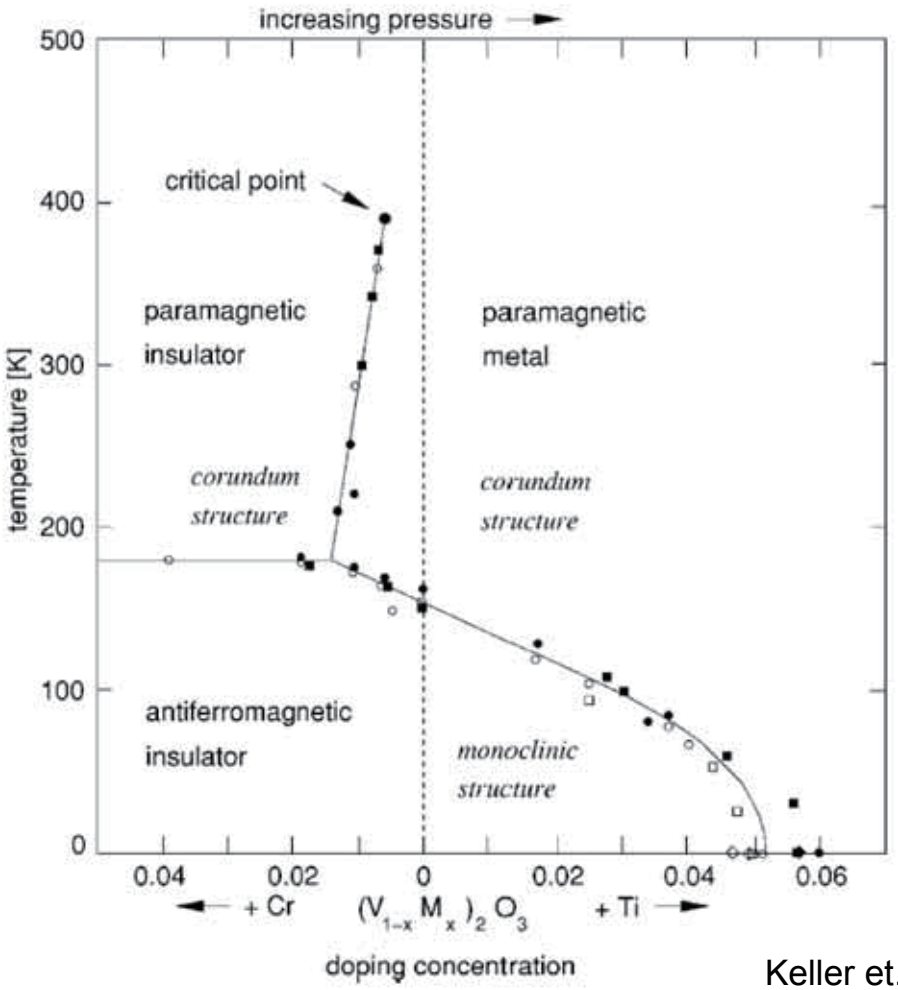
$$P = -iG_0 G_0$$

$$\Sigma = iG_0 W$$

P : Polarization function of RPA

Off-set method, Product-Basis, Parallel Computation etc.

V_2O_3



‡

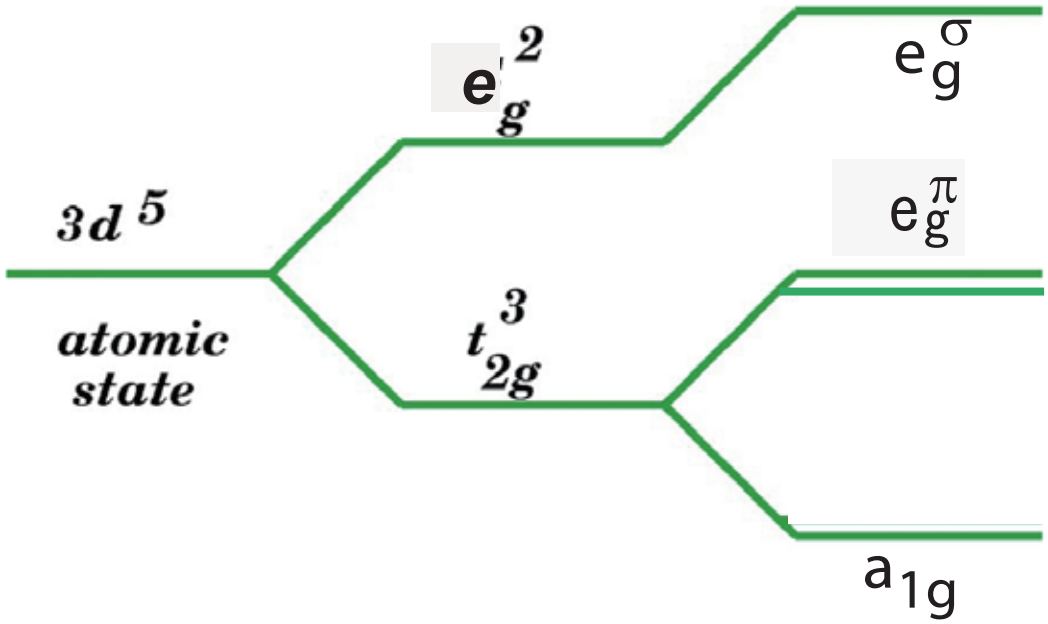
Keller et.al, 2004

PM —— PI　　PM ——AFI

~150K

energy gap=0.35～0.66eV

Vanadium in trigonal symmetric field　d^2



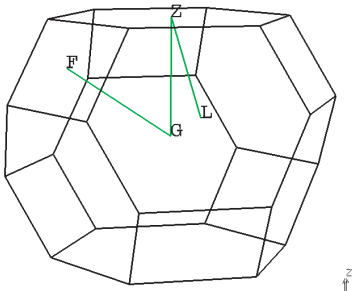
S=1/2　or　M=1.7μ_B

$E(a_{1g})$< or > $E(e_g^\pi)$

What kind of transition

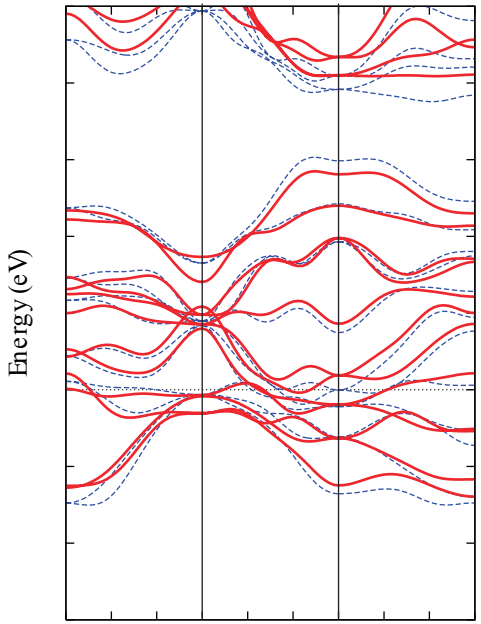
between PM and AFI?

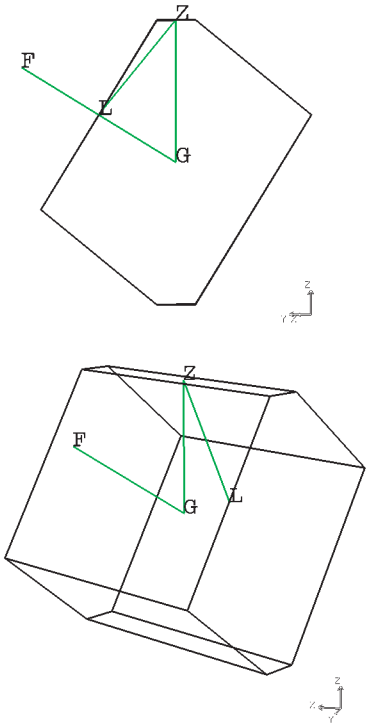
V_2O_3 (U+GWA)

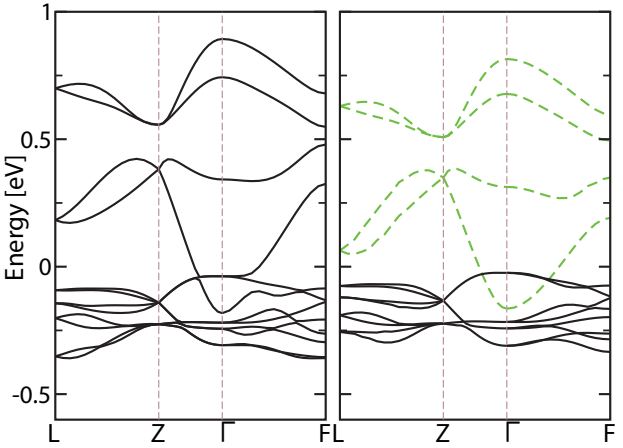


PM

U/J=2.6/0.9 ‡





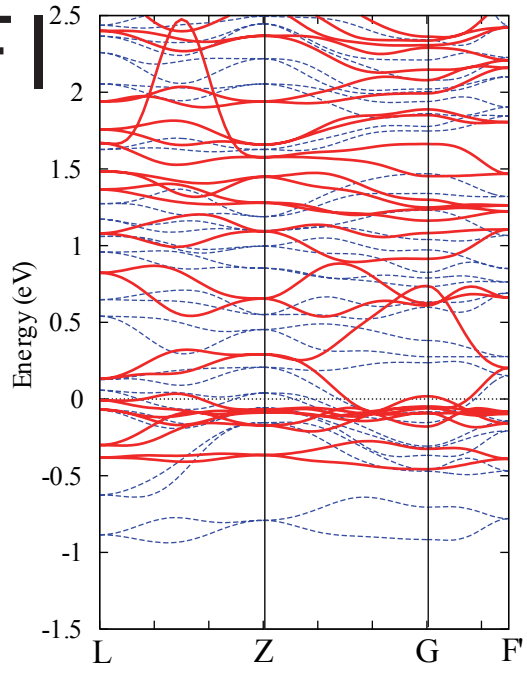


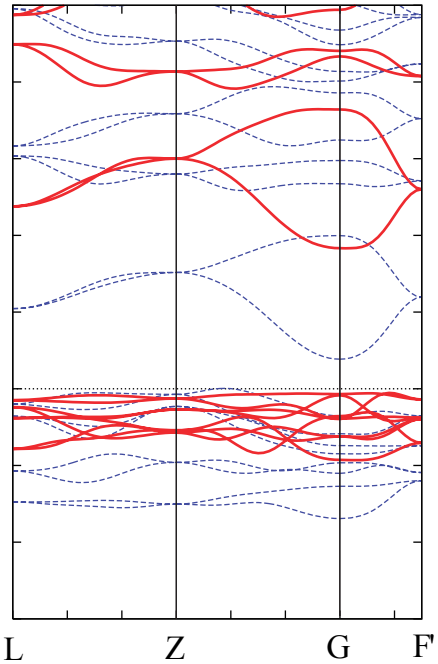
Enhanced Crystal Field Splitting and Orbital Selective Coherence by Strong Correlations in V_2O_3

A.I. Poteryaev,[1] J.M. Tomczak,[1] S. Biermann,[1] A. Georges,[1] A.I. Lichtenstein,[2] A.N. Rubtsov,[3] T. Saha-Dasgupta,[4] and O.K. Andersen[5]

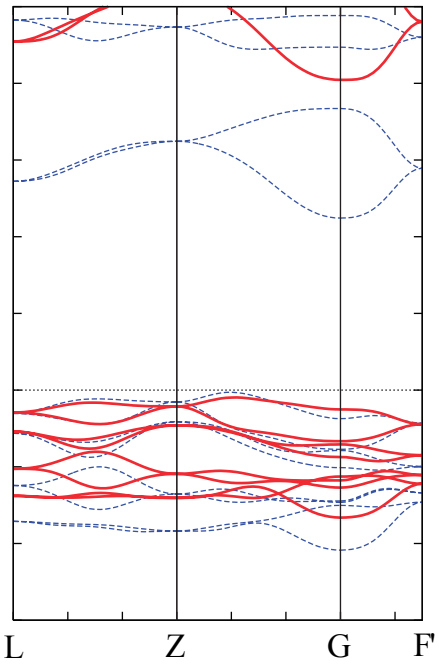
U/J=0/0

AFI





U/J=4.0/0.9



U+GWA

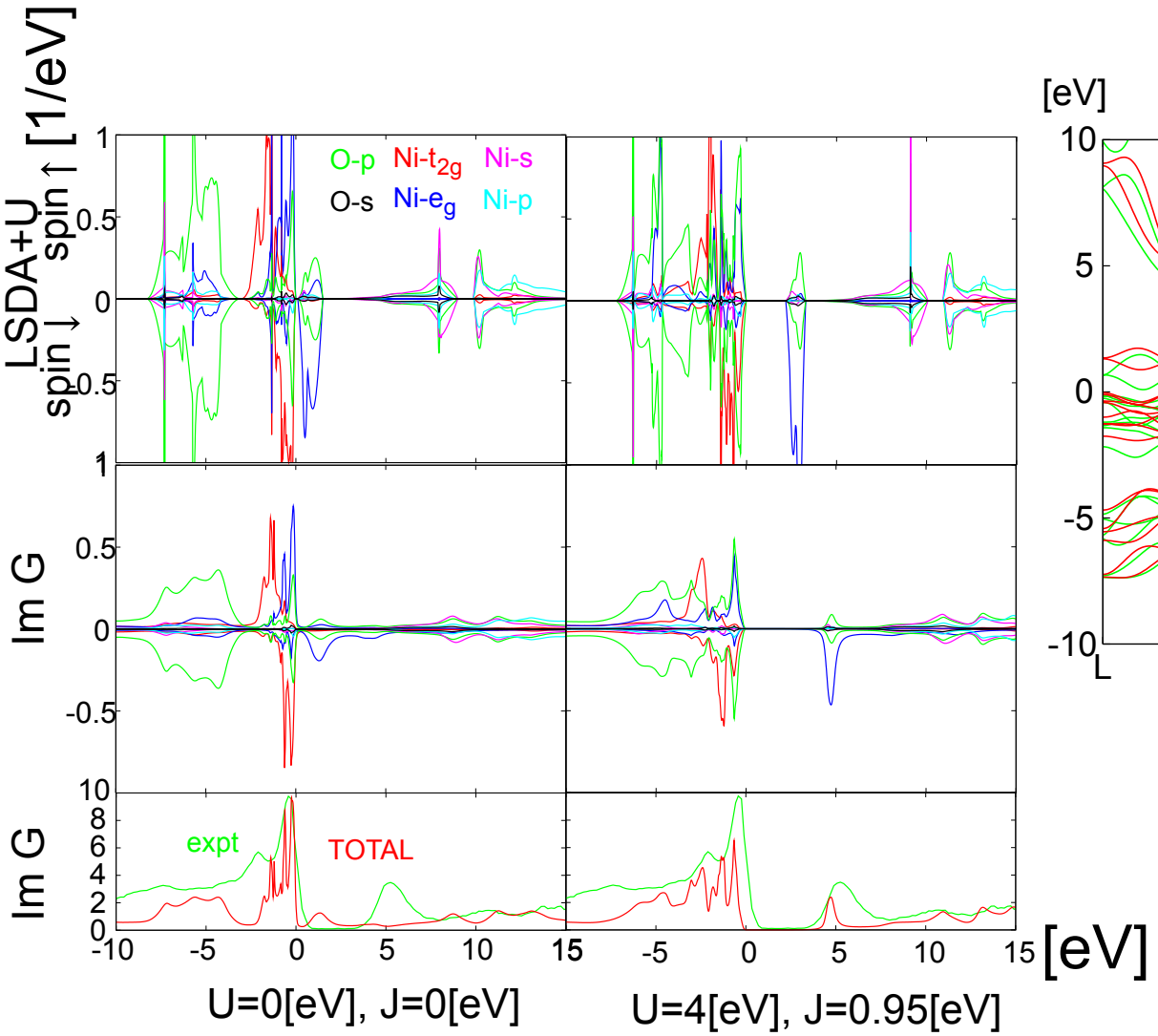
L(S)DA+U

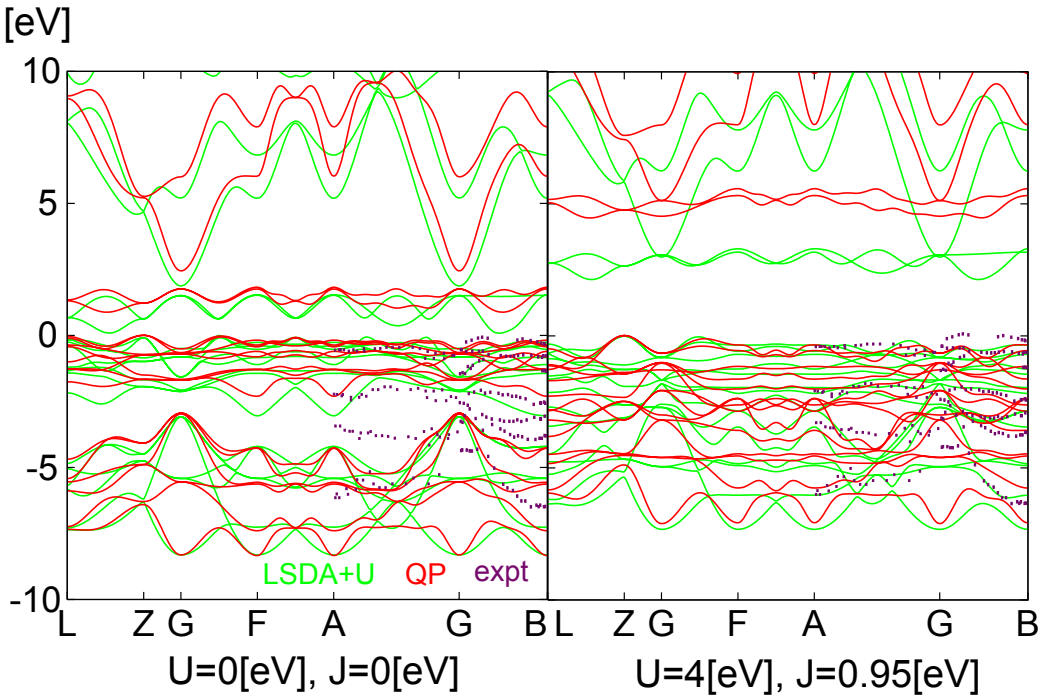
NiO (U+GWA)

Exp:

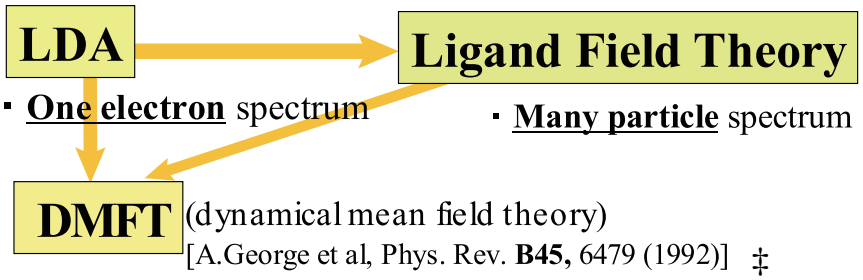
E_g =4.3eV

M =1.9 μ_B



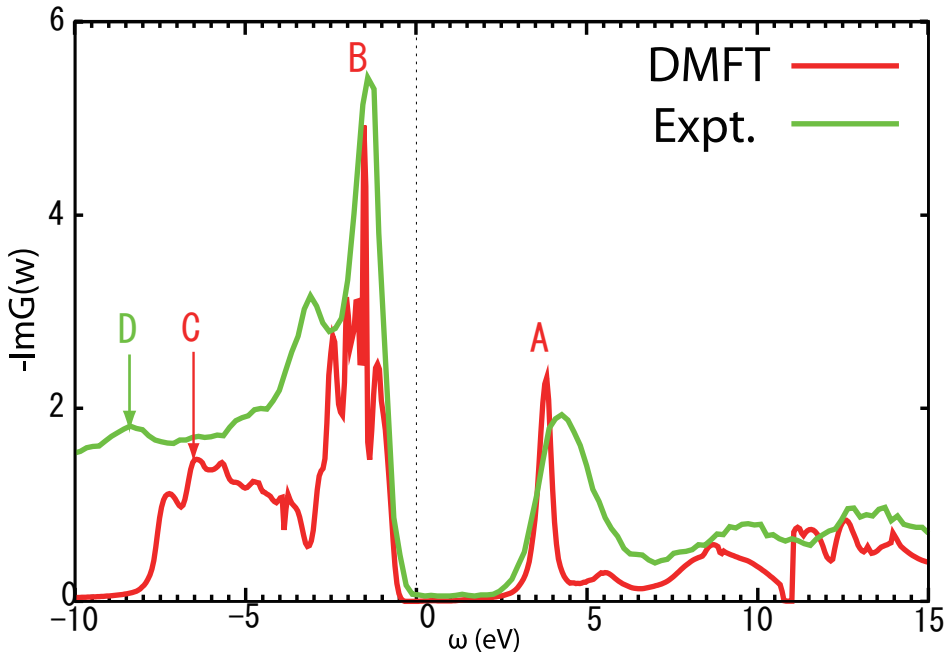


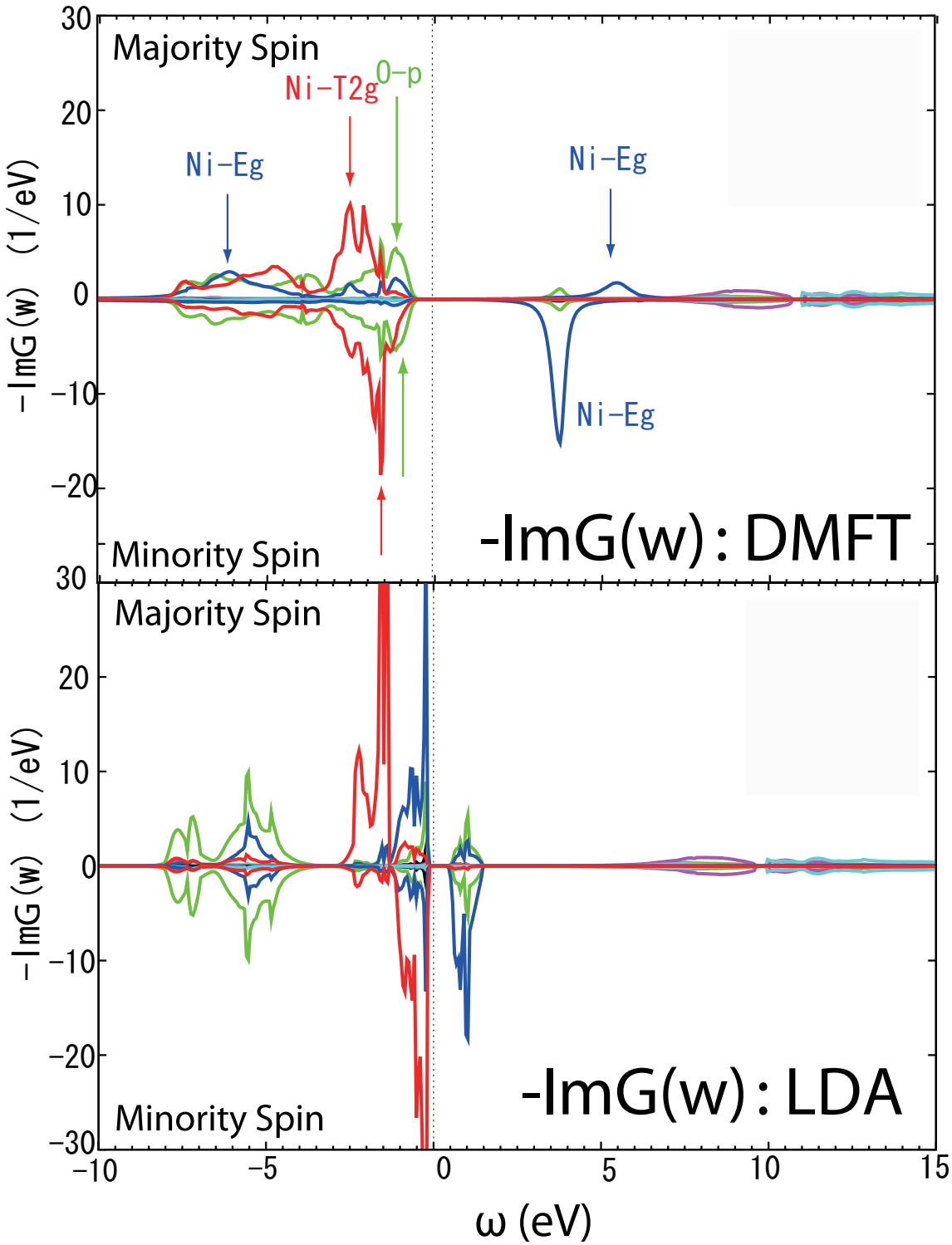
LDA+DMFT (IPT)



$$\Sigma^{(2)}_{m\sigma}(\tau) = -\sum_{m_1 m_2 m_3 \sigma'} (U_{mm_2:m_1m_3} - U_{mm_2:m_3m_1}\delta_{\sigma\sigma'}) U_{m_1m_3:mm_2} \times G^0_{m_1\sigma}(\tau) G^0_{m_3\sigma'}(\tau) G^0_{m_2\sigma'}(-\tau)$$

$$\Sigma(i\omega) = \Sigma^{\mathrm{HF}} + A\Sigma^{(2)}(i\omega)\{1 - B(i\omega)\Sigma^{(2)}(i\omega)\}^{-1}$$





EXACT DIAGONALIZATION of many-body Hamiltonian derived from LDA

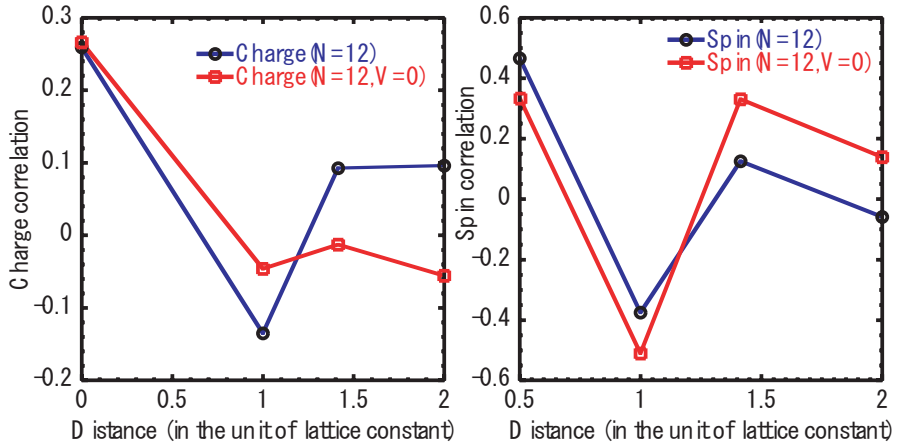
with S. Yamamoto

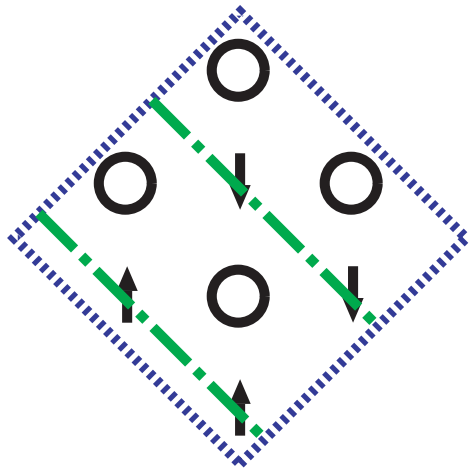
$La_{2-x}Sr_xNiO_6$ (LSNO)

Layered perovskite with stripe order. (0<x<0.5)

x = hole concentration

Antiferromagnetic(AFM) Insulator in the range x<0.9.

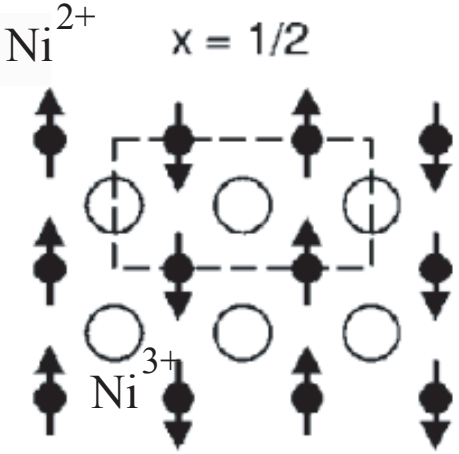




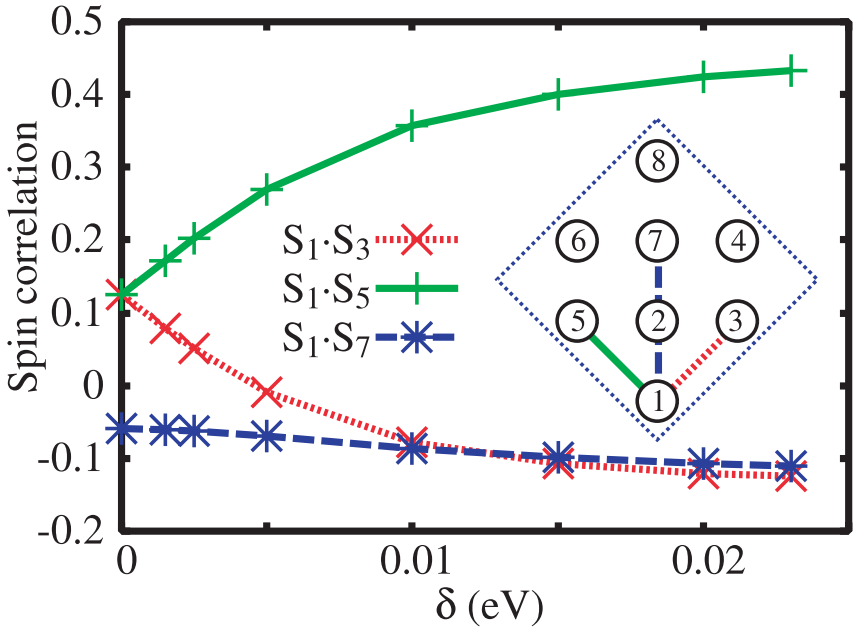
Spin stripe

Ni^{2+} t^6e^2

Ni^{3+} t^6e^1



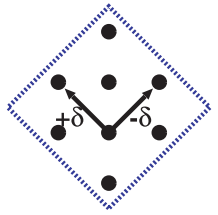
Spin stripe accompanied by anisotropy



V=0.5eV

Néel order : 2nd n.n = 3rd n.n

Orthorhombic anisotropy causes spin stripe



Hopping anisotropy

Off-diagonal Coulomb Interactions → Charge Stripe

Anisotropy of Hopping Integrals → Spin Stripe

Strong coupling between charge and spin fluctuation

密度汎関数理論（基底状態）

単一スレーター行列式（SD）

⇔ 揺らぎ

Linear Method （Muffin-Tin 軌道）

実空間表示 ⇔ Bloch の定理

NMTO, EMTO

大規模系 （Order N method）

励起状態

強相関系

（CI, 相互作用）

空間的揺らぎ GW 近似

⇒ BS-eq. Vertex-corr.

動的平均場近似

時間的揺らぎ

（DMFT, LDA+DMFT）

空間・時間揺らぎ

（GWA+DMFT）

大規模線型方程式の解法

Hamiltonian の構成

ナノスケールシステム

工学教育あるいは大学教育一般について

-専門化の進んだ状況における試み　-

工学教育推進機構の活動

工学専門教育改善の必要性 （1）

1. 工学の拡大、専門の深化：
   工学知の膨張、細分化
2. 地球規模での、複雑で多様な問題の顕現化：
   学際的・融合的な学術
3. グローバリゼーションの進展：
   国際競争と協調

工学専門教育改善の必要性 （2）

- 他大学出身者が大学院生に占める割合：31．4
- 東大の場合：工学系全体　32．3%　専攻別 10% から 59% まで

- 基礎知識の不足を認識（68．3%）
- 学部講義の受講を希望（59．2%）

- カリキュラムの整備を希望（53%）
- 他専攻科目履修を希望（79．2%）

工学教育推進機構
Center for Innovation in Engineering Education

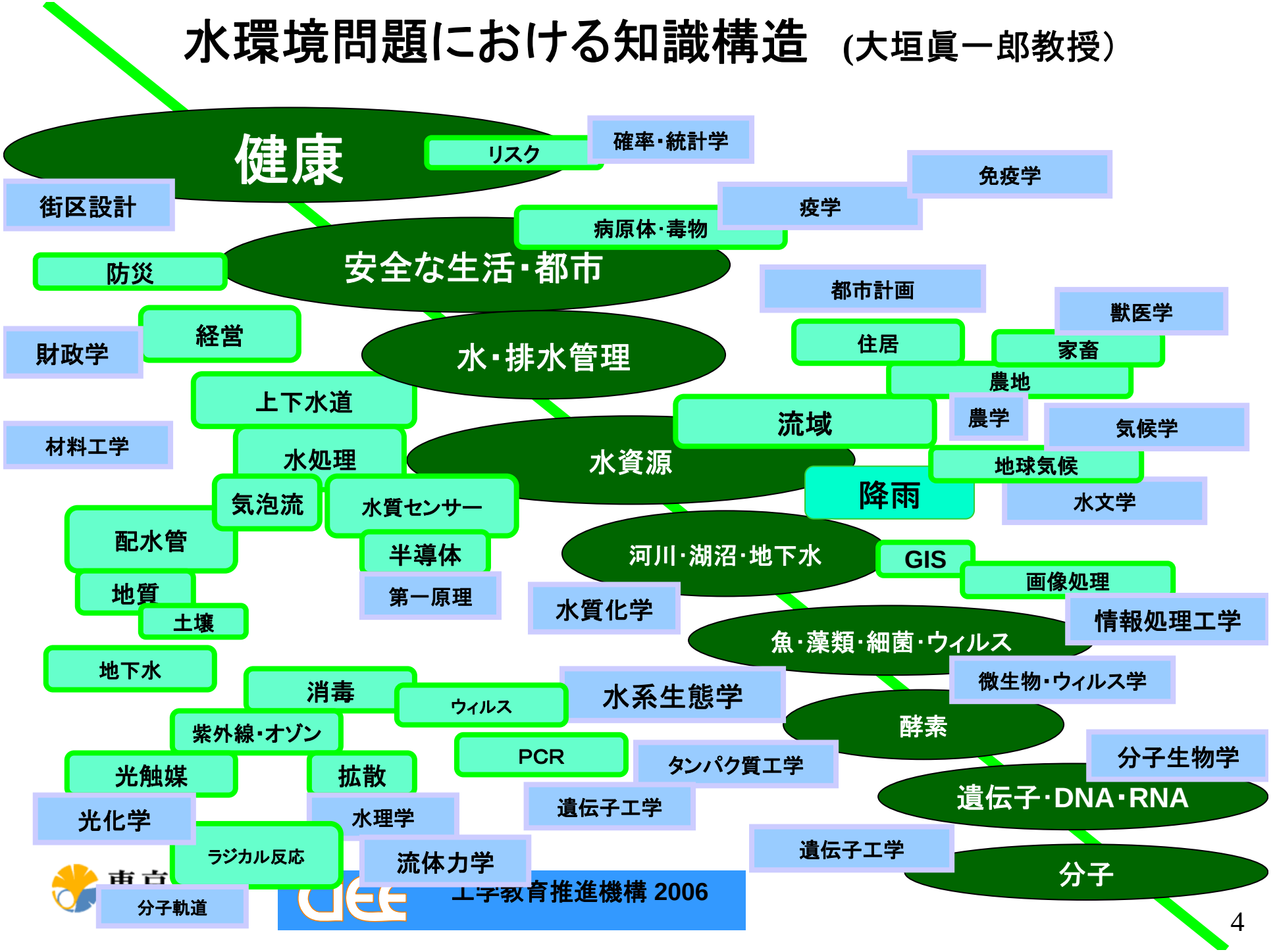
- **2005年、4月1日発足**

- 工学系研究科の２機能（2002年発足）を集結
  - ―「教育プロジェクト室」
  - ―「国際化推進室（GWP）」
- 各々の機能がその活動の枠を広げながら、さらに連携して工学教育改革を推進

工学教育推進機構の設立

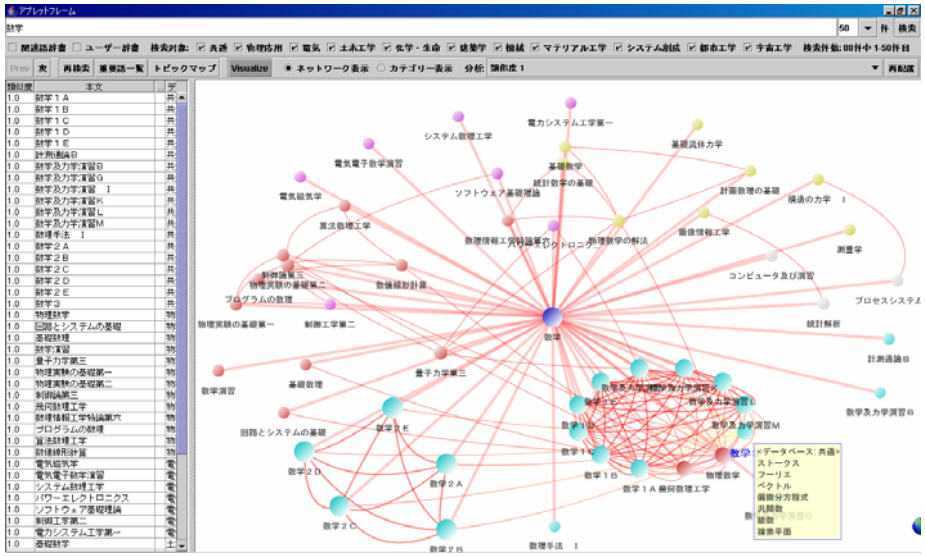
- **工学基礎教育**の充実.
- **専門の壁**を低くする. (inter - discipline)
- Self-orientation, “Tailor-made’’ program

水環境問題における知識構造 (大垣眞一郎教授)



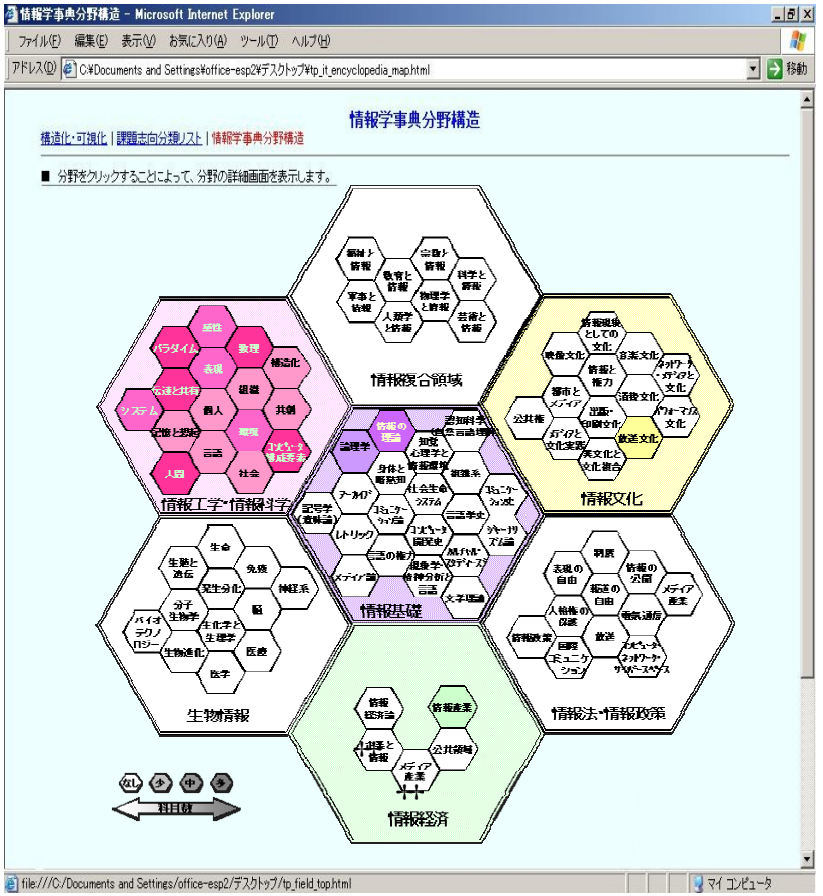
工学知の構造化

Course linkage shown with MIMASearch



美馬秀樹助教授 ‡

課題志向科目（情報関係）構造の具体例



吉田眞教授 ‡

ものづくり実験教育

- 「ものづくり実験ゼミ」と「ものづくりグループ支援」
- ものづくり実験の意義
  - 大学教育の中での
    「もの離れ」「観察、仮説、検証」作業の欠落.
  - 企画、実験、製作、共同作業
    - 情報収集
    - 企画、マネージメント
    - 製作、技術、匠、安全性確保
    - 共同作業、コミュニケーション
    - 発表、レポート、記録
- ものづくり実験工房の建設



もの作り実験「フォーミュラレーシングカーを作る」より

「科学・技術英語」および「スペシャル・イングリッシュ・レッスン」

「科学技術英語」の目的

工学系大学院生の英語発表能力（英語論文執筆、英語口頭発表、英語討論）の増強を図るため、工学系研究科の共通講義として平成15年度夏学期から開講

「スペシャル・イングリッシュ・レッスン」の目的

学部教育における英語教育の増強を目的として、工学部3，4年生を対象として、平成17年度より開始.
GWP室の監督下、複数の英語学校により行う．通常の講義の時間外．学生の負担による受講料（非常に割安）.

GWP室：笠木室長、小野教授、森村講師

皆様、

永い間本当にありがとうございました。

そして、これからもよろしくお願いします。