

# 物質科学の基礎研究における スパコンの必要性

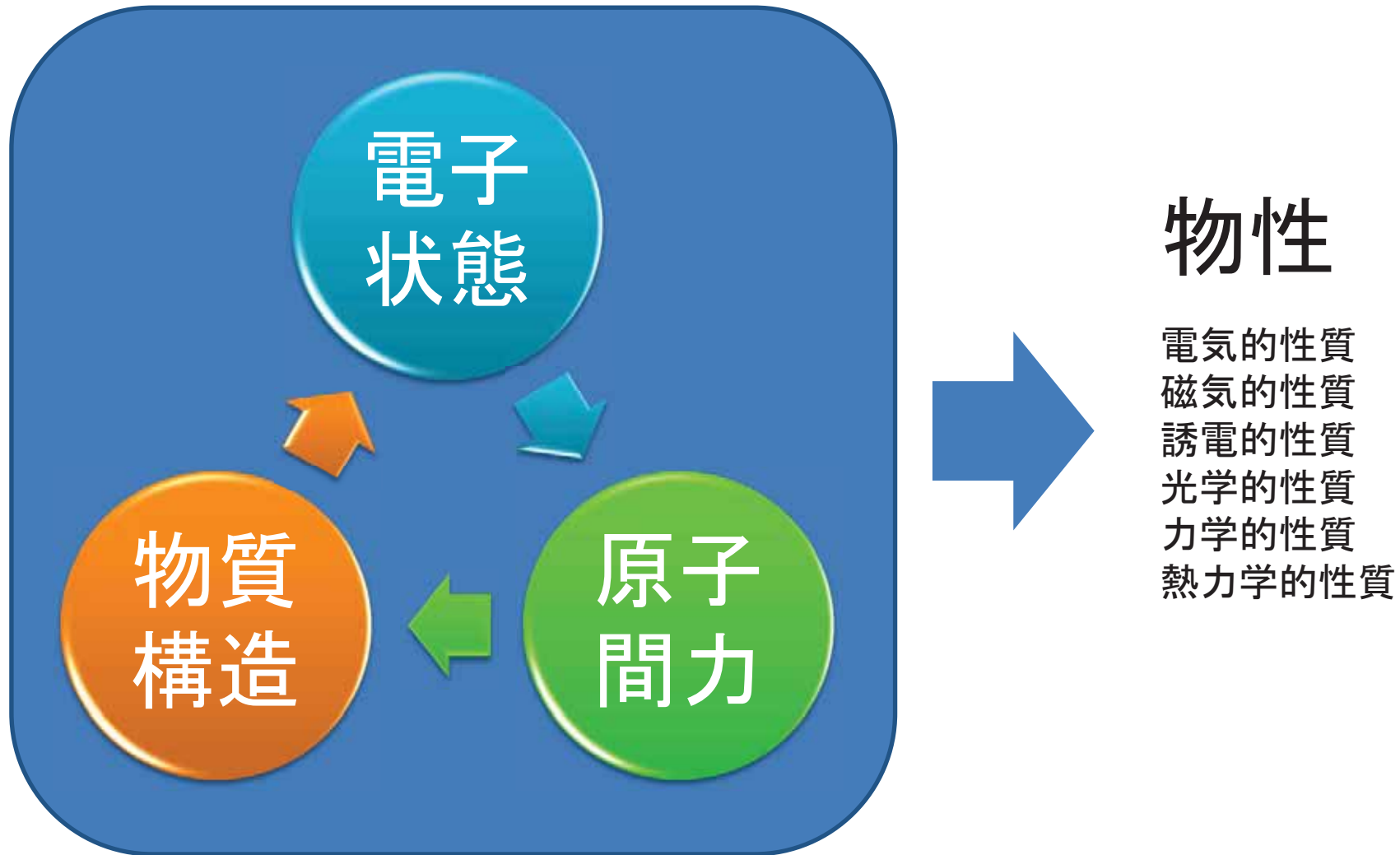
常行真司

東京大学・大学院理学系研究科／物性研究所



計算物質科学イニシアティブ

# 第一原理計算（電子狀態計算、分子動力學）



# 密度汎関数理論 (第一原理計算の基礎理論の一つ)

- 電子の多体問題  $\iff$  平均場の中の1粒子波動方程式
- 全エネルギーと1電子エネルギースペクトル (バンド構造)

$$\left\{ -\frac{\hbar^2}{2m} \Delta + u(\vec{r}) + v_{xc}[\rho(\vec{r})] \right\} \varphi_i(\vec{r}) = \varepsilon_i \varphi_i(\vec{r}),$$

$$\rho(\vec{r}) = \sum_i |\varphi_i(\vec{r})|^2$$

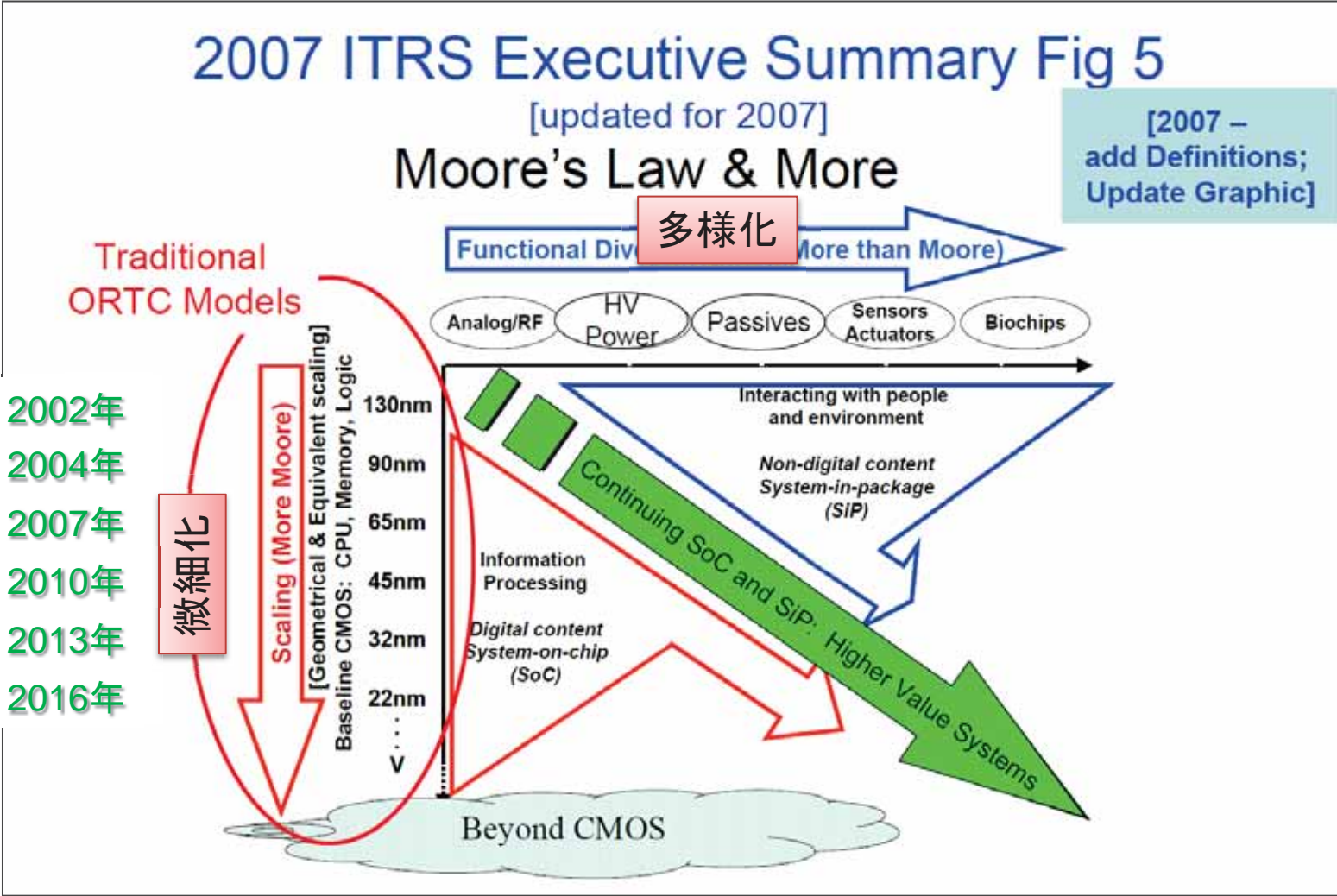
交換相関ポテンシャル

Kohn-Sham 方程式

Hohenberg & Kohn (1964), Kohn & Sham (1965)

*W. Kohn: Nobel Prize in Chemistry, 1998.*

# 将来の半導体デバイス

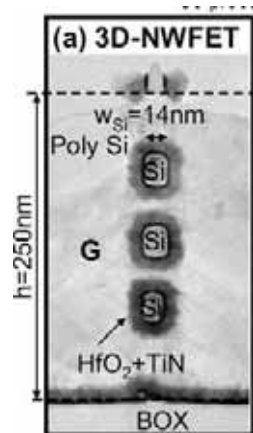
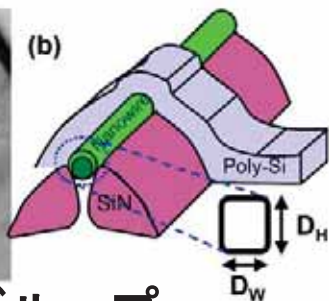
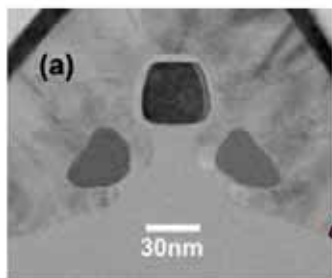
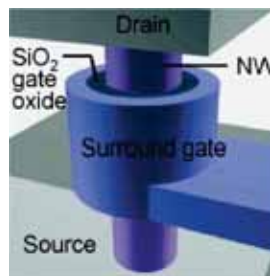
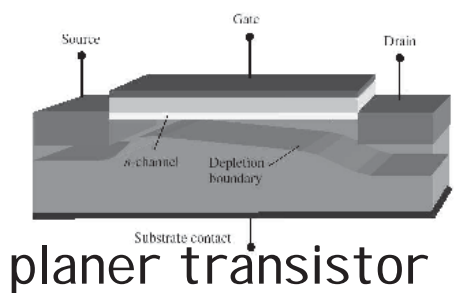


ITRS (国際半導体ロードマップ)

<http://www.itrs.net/>

# シリコン・ナノワイヤー・トランジスター

## 次世代テクノロジーを支える新しいトランジスター



東工大岩井グループ  
(NEDOでの共同研究)  
つくばイノベーションアリーナ  
との共同

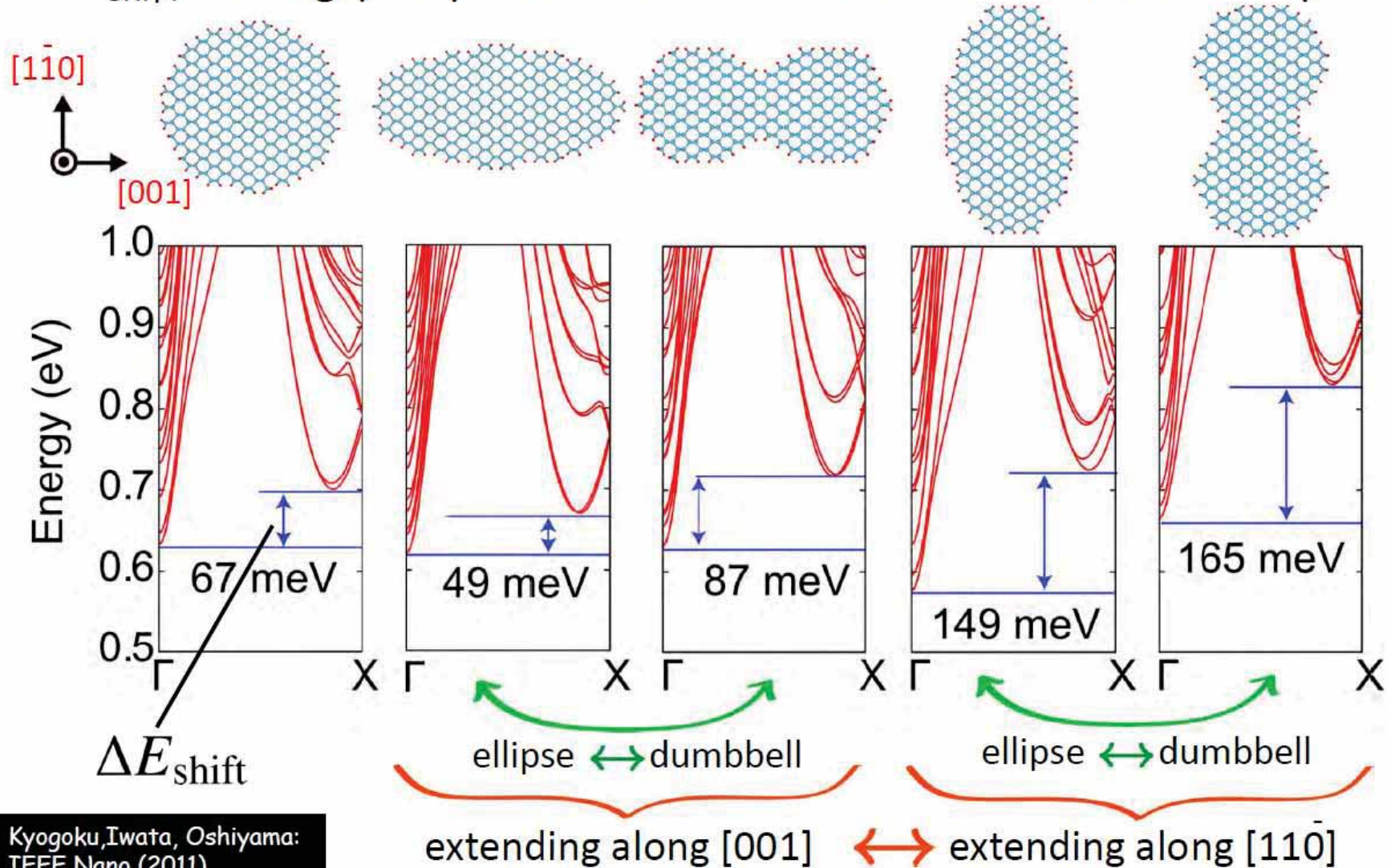
形状、方位、直径、、、  
最適なナノ構造は？  
量子論計算科学の出番



# RSDFTによるSiナノワイヤーの第一原理計算

押山G

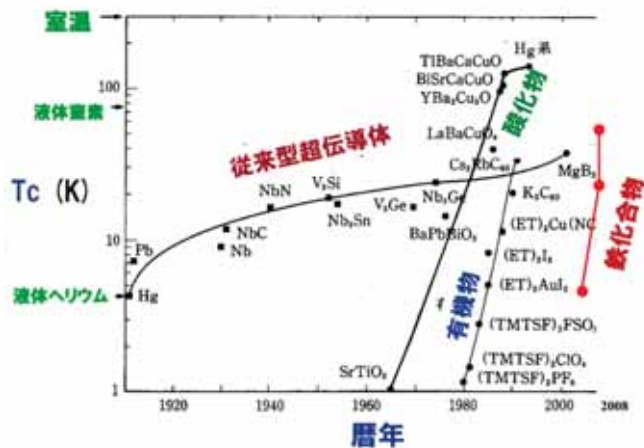
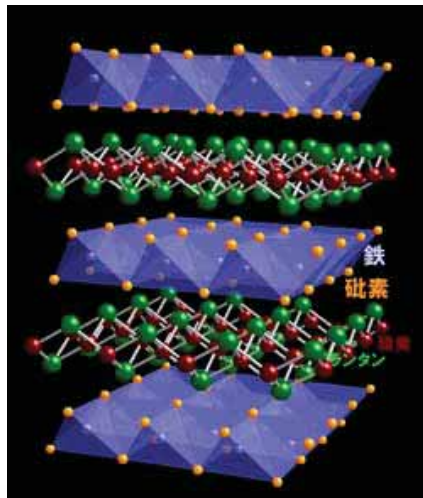
$\Delta E_{\text{shift}}$  strongly depends on the cross-sectional nano-shapes



Kyogoku, Iwata, Oshiyama:  
IEEE Nano (2011)

# 新しい超伝導材料の開発に向けて

鉄ニクタイト系化合物超伝導体  
(東工大 細野グループ, 2008)



母物質のスピン構造

S. Ishibashi, K. Terakura, H. Hosono, 2008

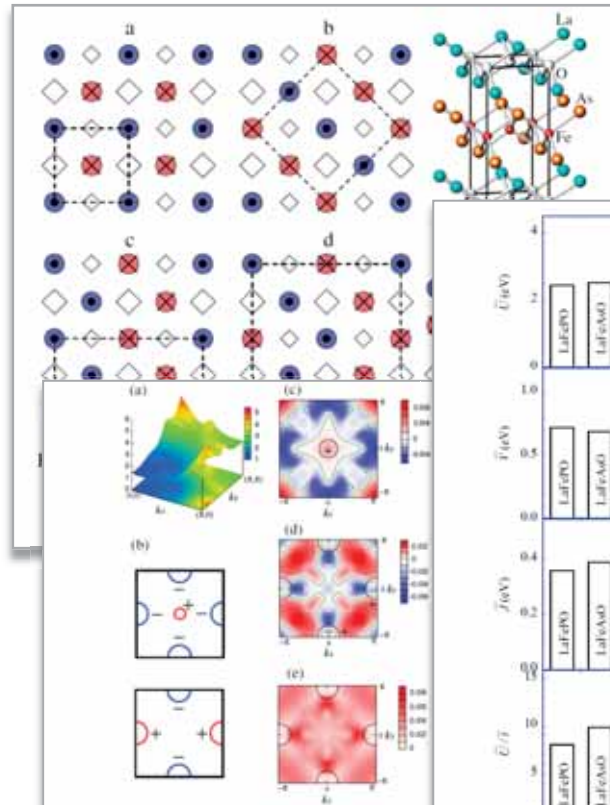


FIG. 2 (color online). RPA result for the spin susceptibility  $\chi_s$ . (a), the gap functions  $\phi_3$  (c) and  $\phi_4$  (d),  $\sqrt{|\phi d^2|}$ .  $U = 1.2$ ,  $U' = 0.9$ ,  $J = J' = 0.15$ ,  $n = 6.1$ , and  $T = 0$  eV. In (c) and (d), the black (green or light gray) represent the Fermi surfaces (gap nodes). In (b), the full extended  $s$ -wave (upper panel) and  $d_{x^2-y^2}$ -wave gaps (lower panel) are schematically shown.

パラメータの物質依存性

T. Miyake, K. Nakamura, R. Arita and M. Imada, 2010

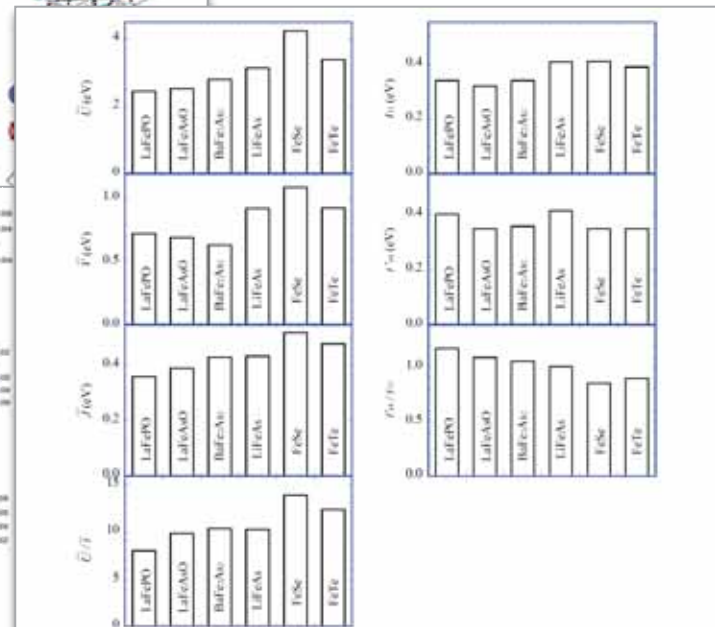
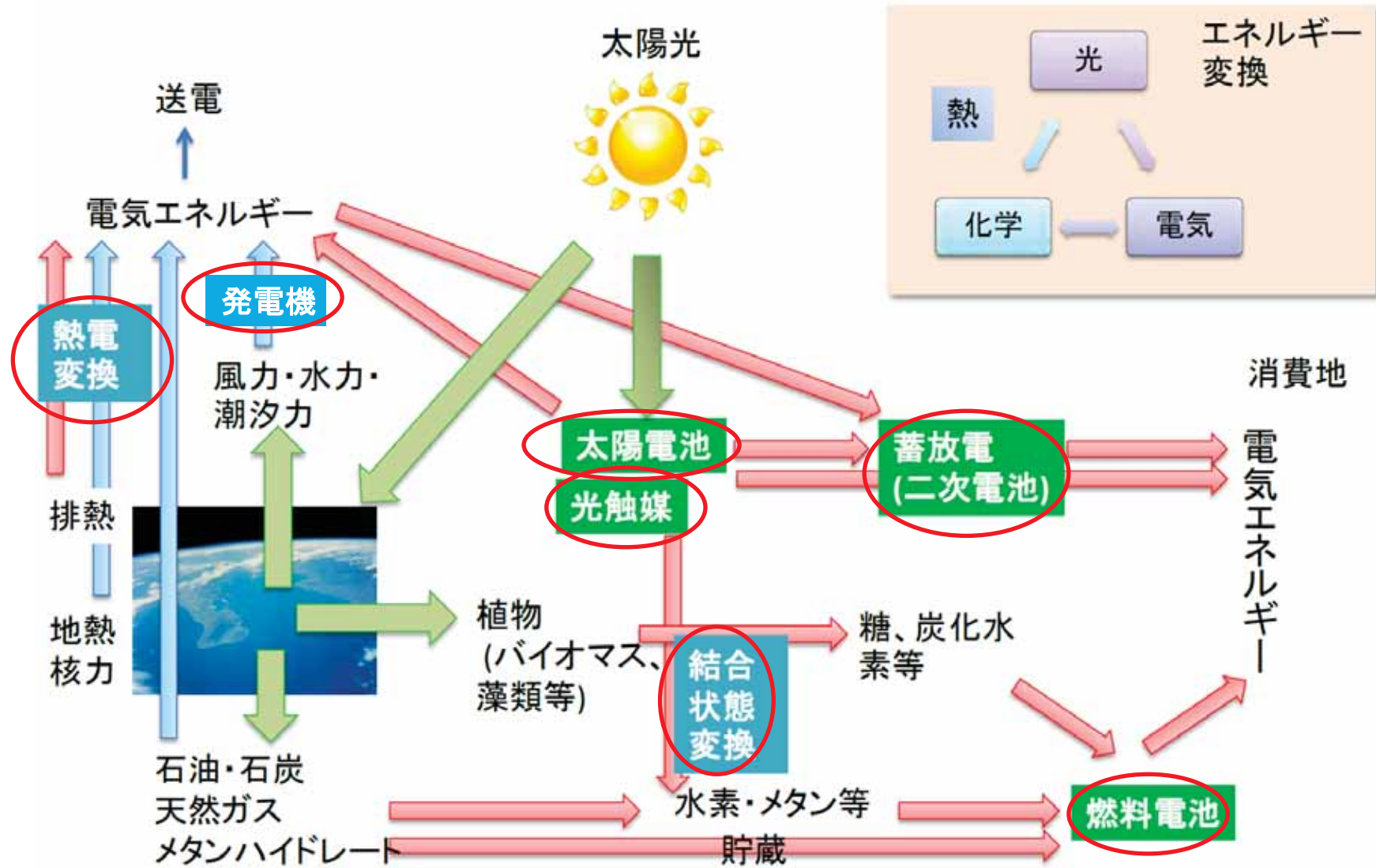


Fig. 7. Material dependence of parameters in  $d$  model. The average of the onsite effective Coulomb interactions ( $\bar{U}$ ), the average of  $d$  orbitals effective Coulomb interaction between the neighboring Fe sites ( $T$ ), the average of the onsite effective exchange interactions ( $J$ ), the maximum value of the transfer integrals between the neighboring Fe sites ( $J_{ij} = J_{11}(1/2, -1/2, 0)$ ) and between the next-nearest neighbor ( $J_{ij} = J_{42}(1, 0, 0)$ ),  $\bar{U}/U$ , and  $J_{41}/J_{11}$  are compared. The subscripts of  $J_{11}$  and  $J_{41}$  are orbital indices, 1 for  $xz$  and 4 for  $yz$ .  $\bar{U}$  is the orbital average of the largest nearest  $d-d$  transfer integrals.

第一原理モデルハミルトニアンによる超電導理論

K. Kuroki, S. Onari, R. Arita, H. Usui, Y. Tanaka, H. Kontani and H. Aoki, 2008

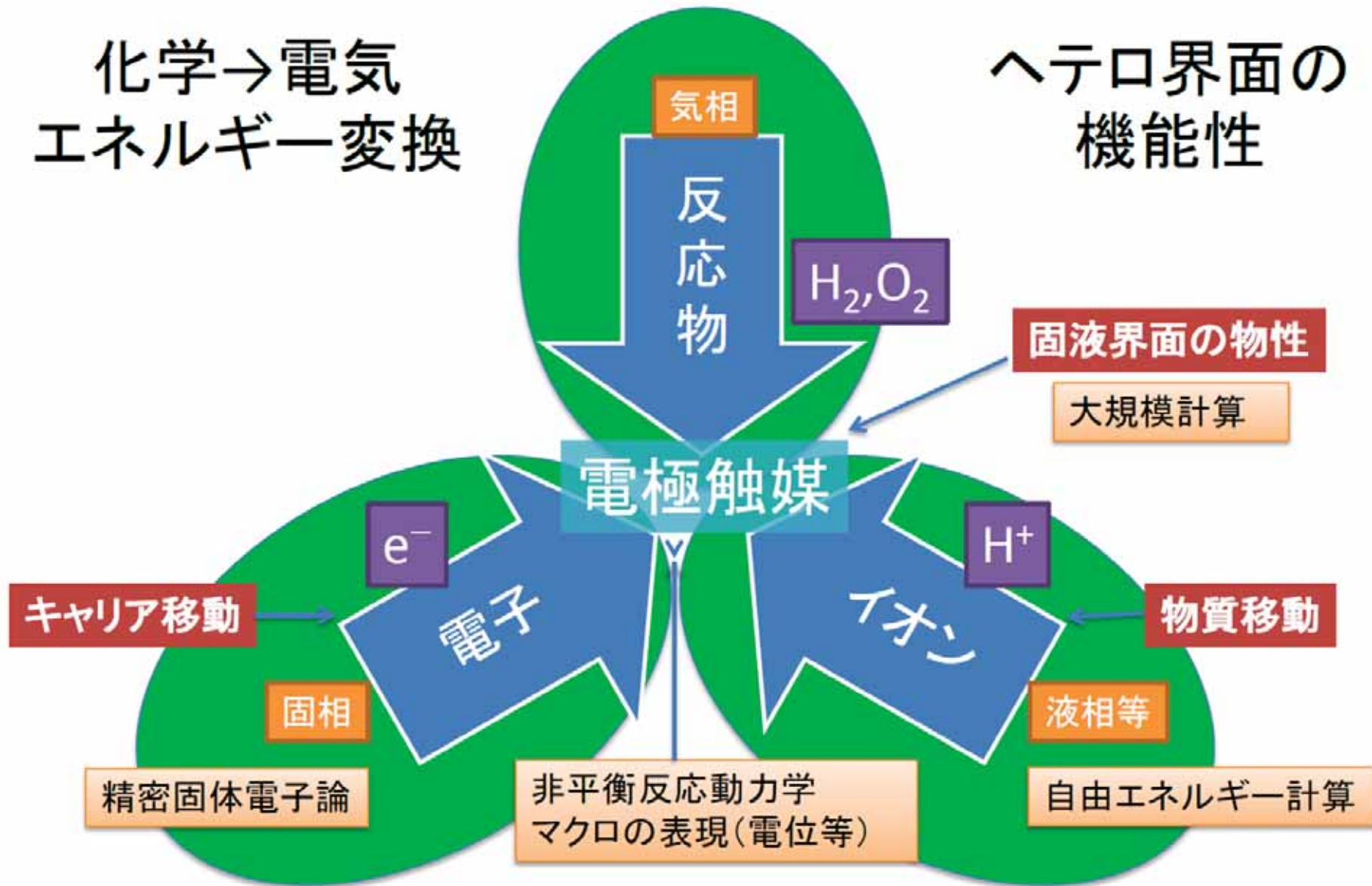
# エネルギー問題



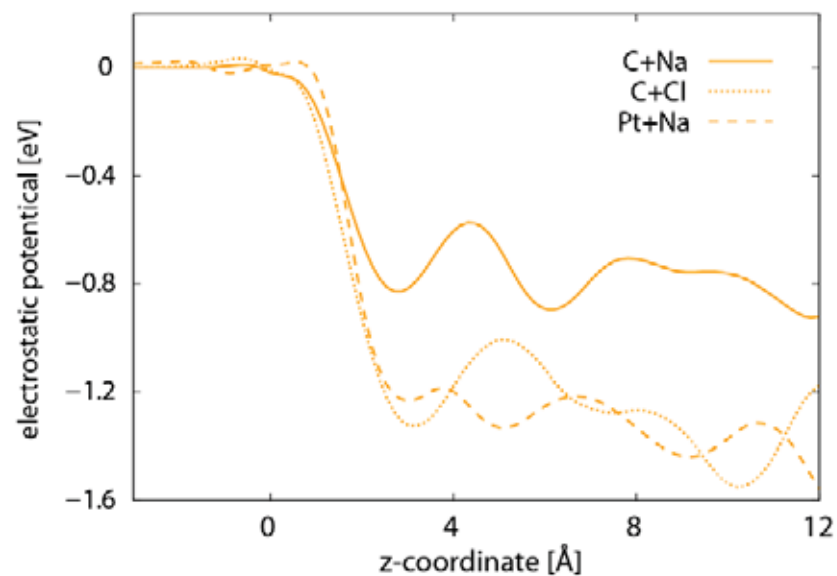


化学→電気  
エネルギー変換

ヘテロ界面の  
機能性



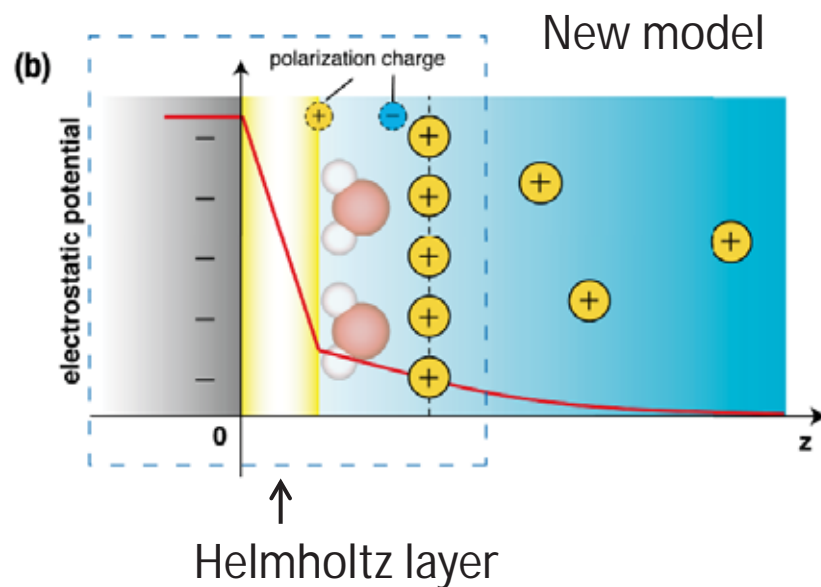
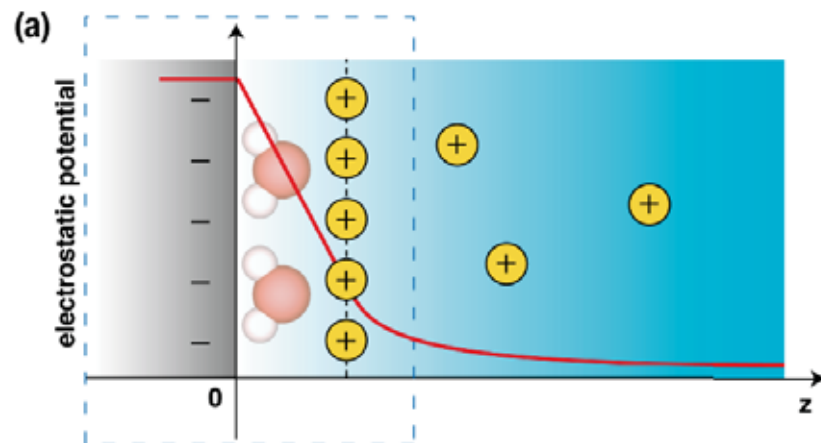
# 電気二重層



FPMD + ESM

Y. Ando, Ph.D. Dissertation (2012)

Conventional model



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# 今後の課題の例

# 太陽電池: Staebler-Wronski effect

Appl. Phys. Lett. 31, 292 (1977).

## Reversible conductivity changes in discharge-produced amorphous Si<sup>a)</sup>

D. L. Staebler and C. R. Wronski

RCA Laboratories, Princeton, New Jersey 08540  
(Received 9 May 1977; accepted for publication 17 June 1977)

A new reversible photoelectronic effect is reported for amorphous Si produced by glow discharge of SiH<sub>4</sub>. Long exposure to light decreases both the photoconductivity and the dark conductivity, the latter by nearly four orders of magnitude. Annealing above 150°C reverses the process. A model involving optically induced changes in gap states is proposed. The results are discussed in terms of the physical nature of the material and for its applications in solar cells. The reproducibility of measurements on discharge-produced Si.

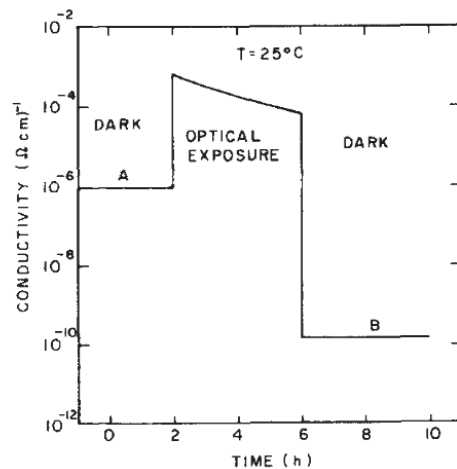
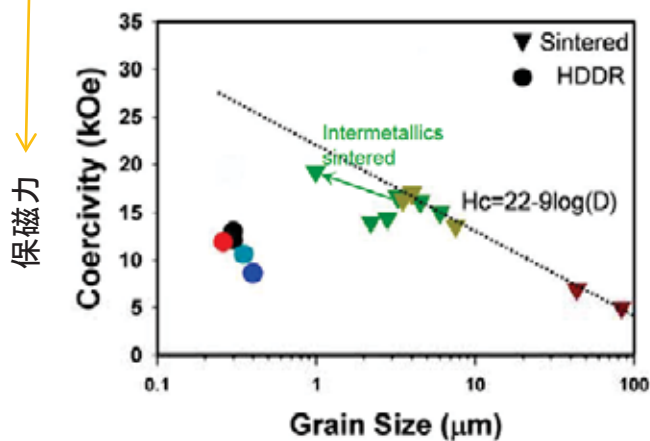
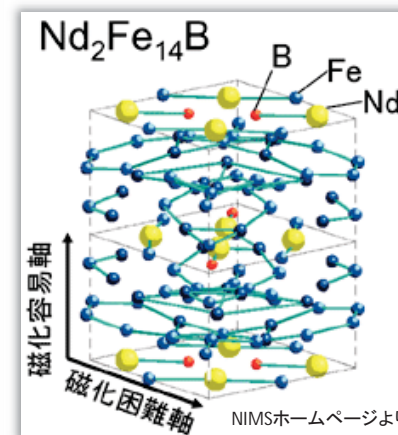
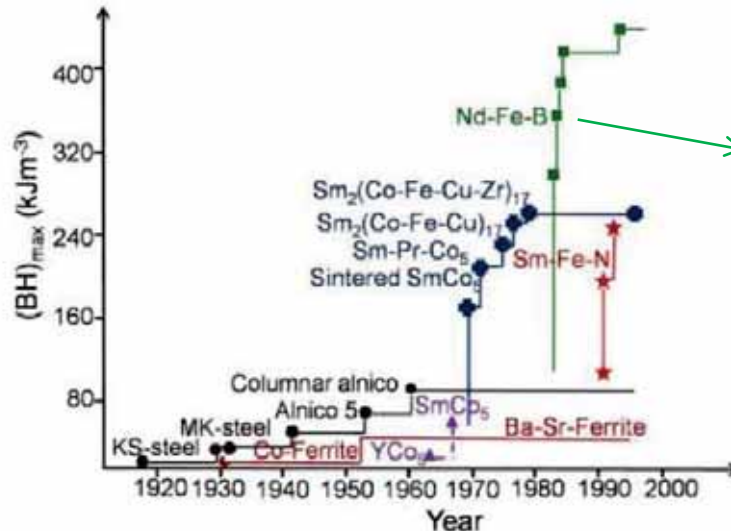
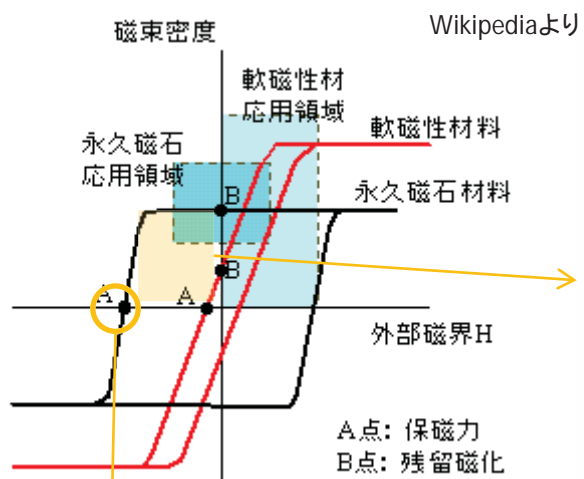


FIG. 1. Conductivity as a function of time before, during, and after exposure to ~ 200 mW/cm<sup>2</sup> of light in the wavelength range 6000–9000 Å.

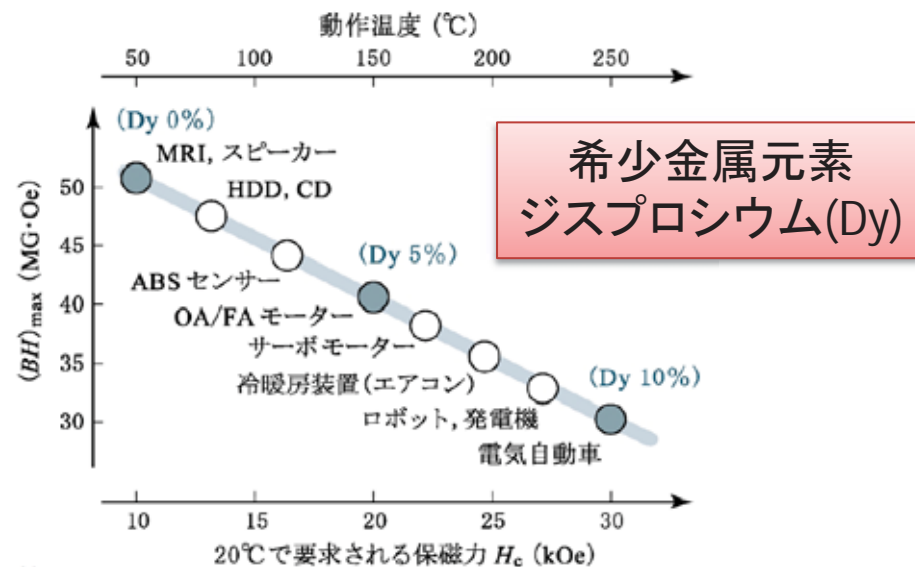
The screenshot shows the homepage of 'Alternative Energy' with a navigation bar including 'Home', 'Energy News', 'Green Jobs', 'Events', 'Directory', and 'Search'. A main article titled 'Economical Solar Panels to Yield More Energy' is featured, dated July 26th, 2010. The article text discusses research at TU Delft to improve amorphous solar panels. A sidebar on the left contains advertisements for 'Remote Hybrid Helper', 'Components at Digi-Key', and 'Green Silicon Carbide'. A small image of a solar panel array is visible on the right side of the article.

<http://www.alternative-energy-news.info/economical-solar-panels-more-energy/>

# 磁石

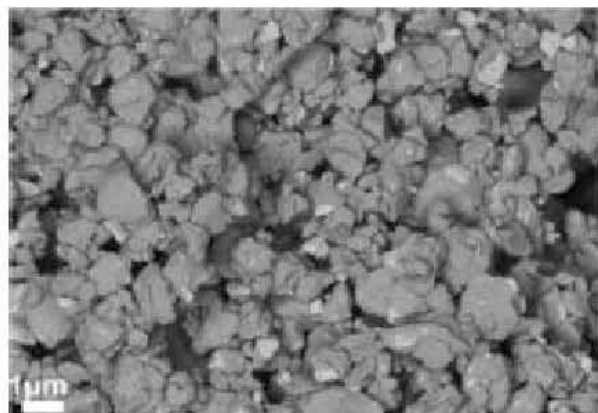


H. Sepheri-Amin et al. Scripta Mater. 65, 396 (2011).

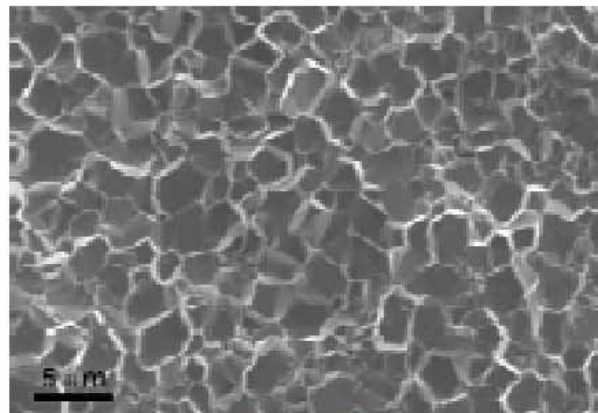




# 磁石

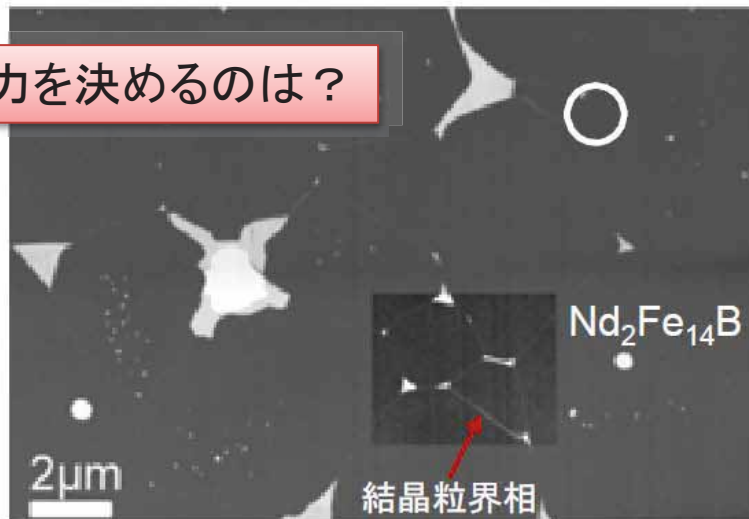


→  
焼結



$$D_{GB} \sim 1.5 D_{\text{powder}}$$

保磁力を決めるのは？



# スパコンの必要性

↑  
計算結果の信頼性・予言力

第一原理計算の「ヤコブの梯子」



↑  
計算量・メモリー

多体問題の理解

実験の補完

物質設計

→  
システムサイズ・サンプル数・長時間ダイナミクス