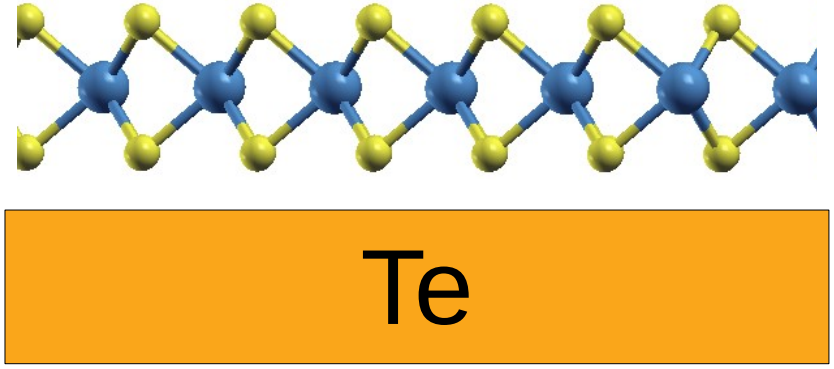
2019 研究テーマ

方法	題目	共同研究
DFT	Schottky barrier in 2D-transistor material: Te / MoTe2 interface	青木研
DFT	Exchange bias system. Structure and magnetism of Mn islands on Fe(110)	山田研
DFT+ scattering	Molecular coupling effect on ARPES of organic molecules: Mn phthalocyanine	解良研
DFT+ scattering	ARPES of hexagonal boron nitride/Cu(111)	Jülich (D)
Program-ming	Calculation of scattering matrix for arbitrary potential shape	富山大
Multiplet	Theory of X ray absorption spectra from transition metal atoms in chiral molecules	
Statistical mechanics	Thermodynamics of alloys from pair-distribution function / X-ray diffraction data	Dijon (F)
DFT-AI	Make algorithm for finding adsorption site from charge density w/o SCF calculation	先進ｾﾝﾀｰ

Schottky barrier in 2D-transistor material: Te / MoTe2 interface



- MoTe2 = new 2D semiconductor
- Laser irradiation → doping, phase transition
- Strong laser → phase separation Te-Mo
  → formation of semi-metallic Te
  → reduction of Schottky barrier at electrode
- Te / MoTe2 interface structure unknown
  → ab initio modeling

Structure and magnetism of islanded Mn/Fe(110)

背景:

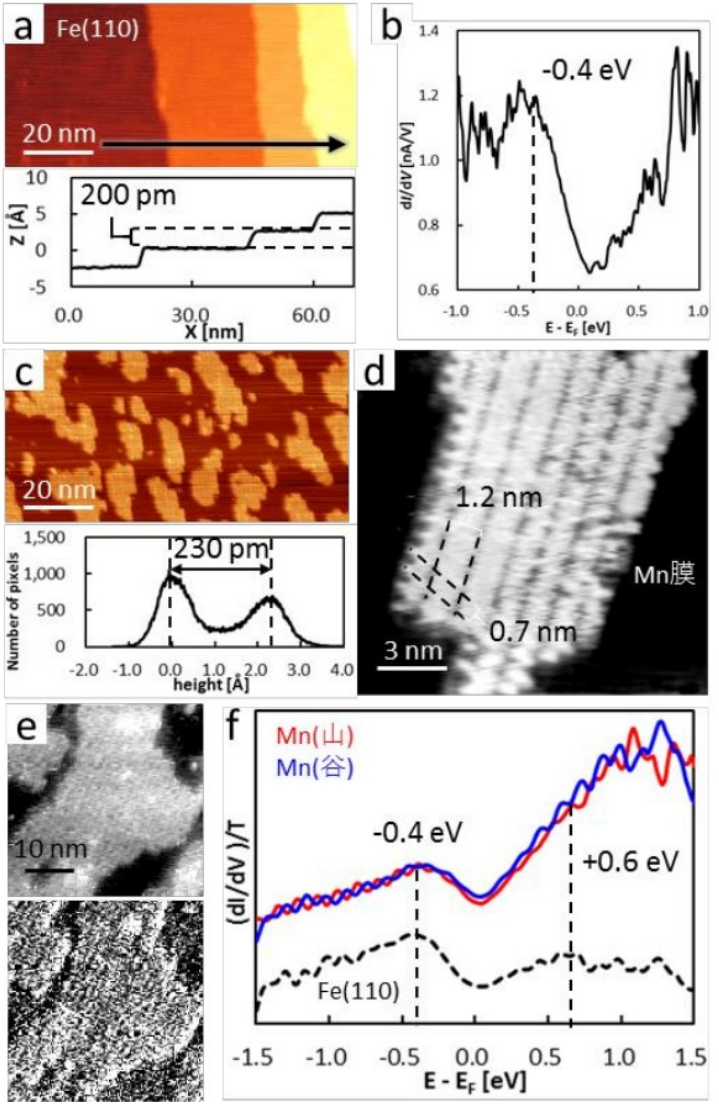
山田先生が Fe(110) 基板に吸着された Mn 一層の薄膜・ナノアイランドを作成した。

強磁性体・反強磁性体の界面はスピン Valve 等の spintronics デバイスで使われる。

課題:

１） Mn 一層の薄膜験の構造・電子状態・スピン構造を DFT で計算する。

２）ナノ島の安定さ、新構造を求める。



林氏（山田研）卒論

Europhys. Lett., 46, 231-237 (1999)
Parallel, antiparallel and no magnetic coupling in submonolayer Mn on Fe(110)
O. Rader , C. Pampuch, W. Gudat, A. Dallmeyer, C. Carbone and W. Eberhardt

In this letter, we report on three intriguing coupling effects occurring in the same system
and sample: i) absence of coupling in the low-coverage limit, which has never been reported
before, ii) parallel coupling from 0.4 to 2 ML, contrasting our findings on the (100) surface of
antiparallel coupling vanishing at 1 ML, and iii) a surprising reversal to antiparallel coupling
by oxygen dosage. We will discuss explanations for the first two in detail, the oxygen effect,
however, remains much less understood.

J. Phys.: Condens. Matter 28 (2016) 326001
doi:10.1088/0953-8984/28/32/326001
Noncollinear magnetism of Mn nanowires on Fe(1 1 0)
R N Igarashi , I P Miranda, L T F Eleno, A B Klautau and H M Petrilli

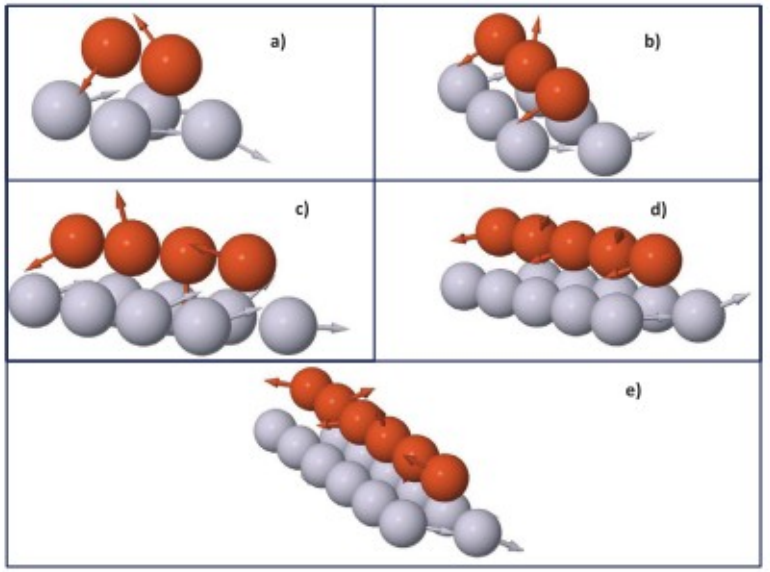


Figure 5. Noncollinear magnetic configurations for Mn nanochains deposited on Fe(1 1 0): (a) Mn_2; (b) Mn_3; (c) Mn_4; (d) Mn_5; (e) Mn_6. The orange (dark) and gray (light) spheres represent Mn and Fe atoms, respectively. The arrows indicate the local spin moment directions.

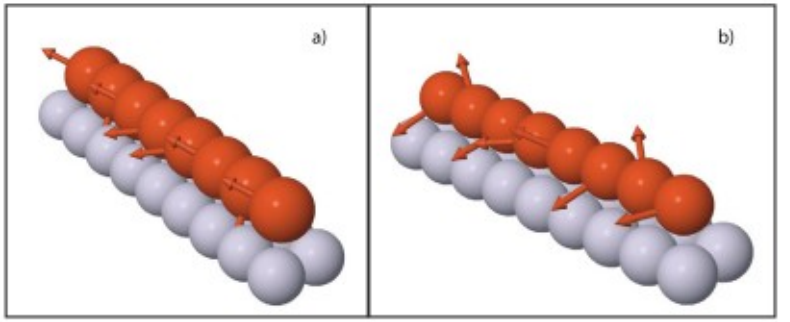
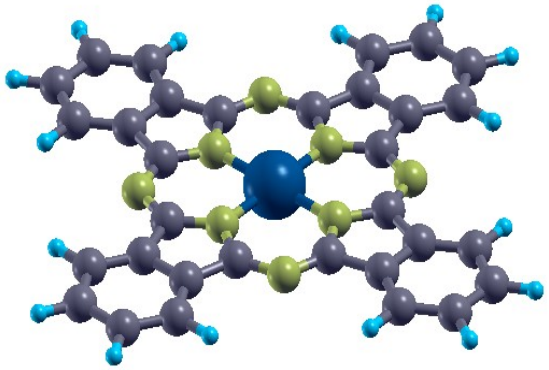
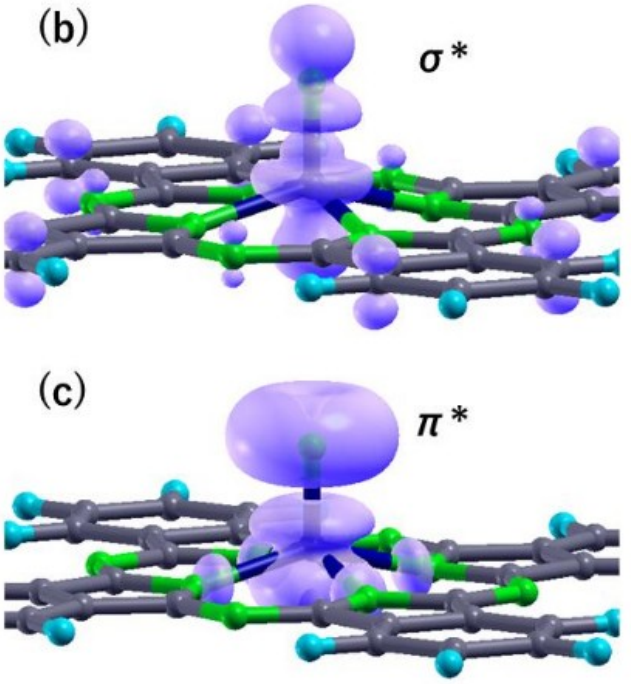


Figure 6. Noncollinear magnetic configurations for Mn_8/Fe(1 1 0) (a) without and (b) with spin–orbit coupling. The orange (dark) and gray (light) spheres represent Mn and Fe atoms, respectively. The arrows indicate the local spin moment directions.

ARPES of 2-layer Mn-phthalocyanine

Molecular coupling effect on ARPES of organic molecules:
Mn phthalocyanine





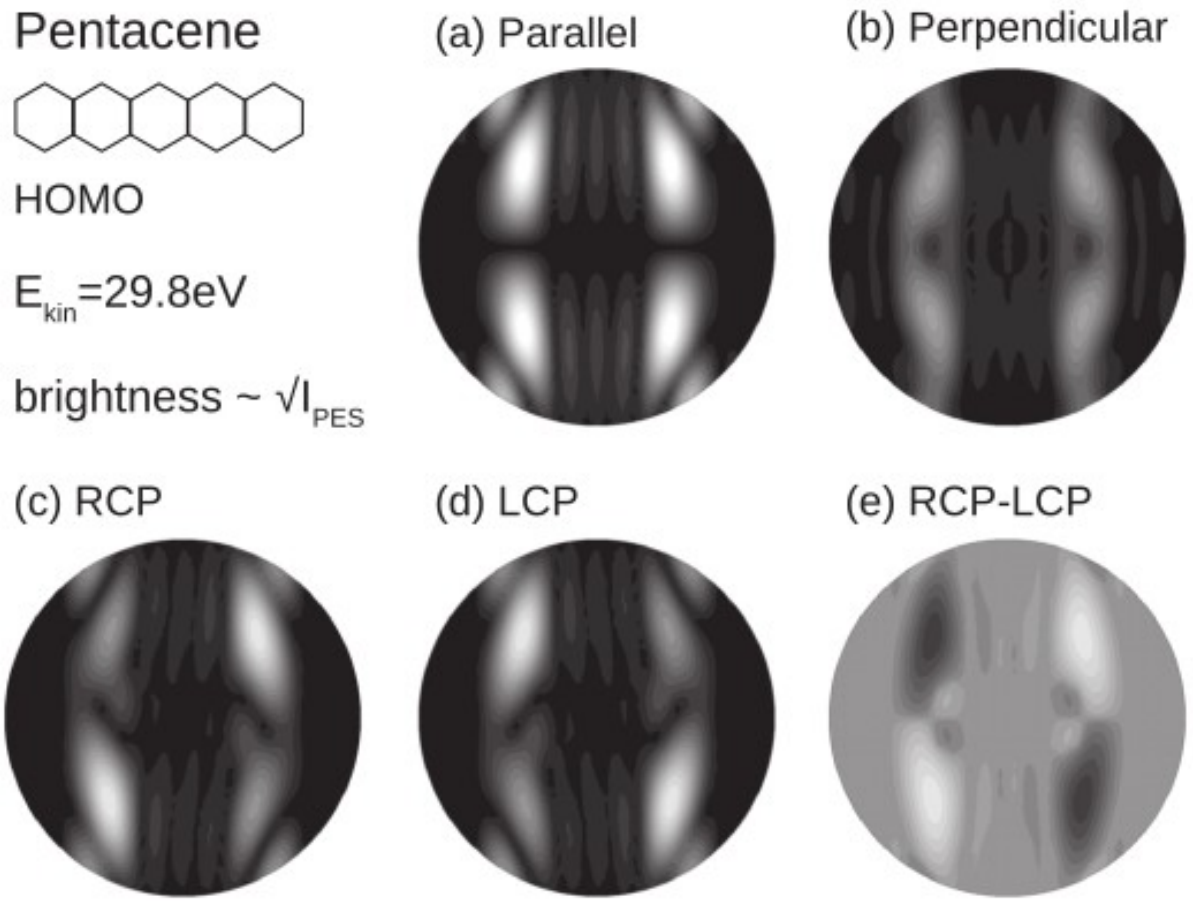
To do:

1) reproduce 1 monolayer → 石川さんの修論
2) make model for 2 layer
   Compute ARPES as a function of structure

Calc: Gaussian + Multiple scattering program (PK)

Exp: 良解先生

Refs 石川さんの修論
P Krüger, J. Phys. Soc. Japan 87, 061007 (2018)



P Krüger, J. Phys. Soc. Japan 87, 061007 (2018)

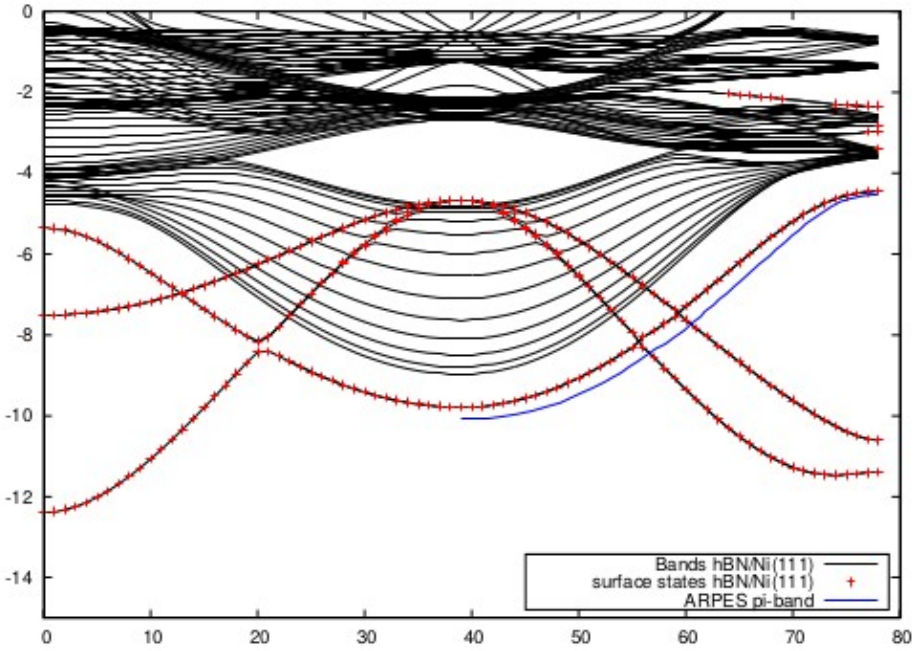
ARPES h-BN/Cu(111)

Objective: energy dependence of sigma and pi bands.
Comparison of different methods:

- plane wave approximation (VASP → 前川、小野さん)
- multiple scattering calculation (with LMTO band structure/potentials → 藤方さん)

Confidential data

h-BN/Ni(111)



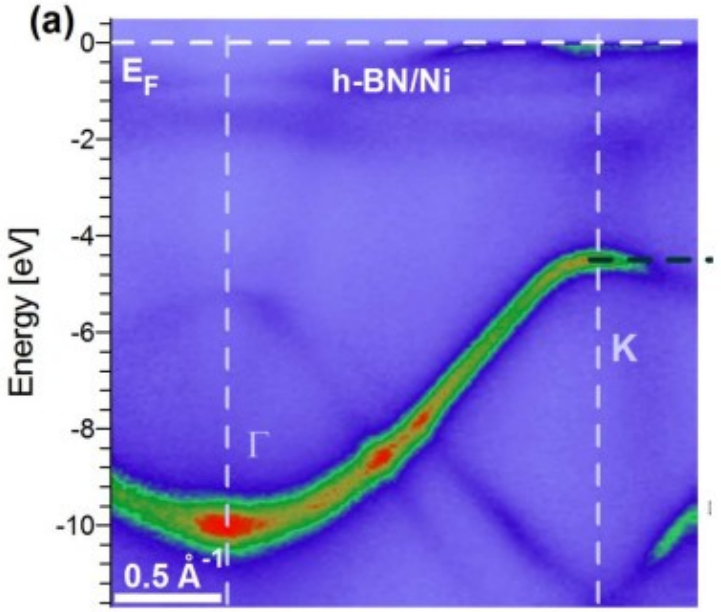
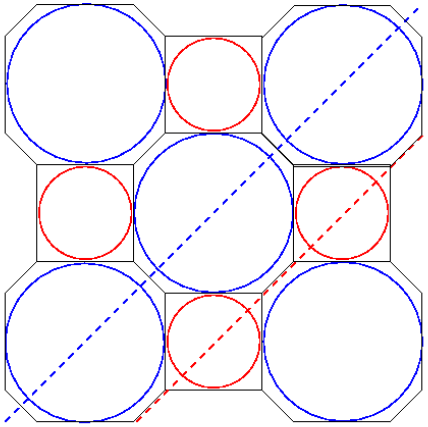


Figure 4.4: left: Comparison between ARPES experimental data (blue line) and theoretical (red dashed line) surface states. Black curves represent the whole theoretical band structure (with inner states). right: ARPES band structure of h-BN/Ni

Study of the Electronic Structure of hexagonal Boron Nitride on Metals Substrates
Paul Giraud, Master thesis, Univ Lille, 2003.

nano-bio.ehu.es/files/paulgiraud_masterthesis.pdf

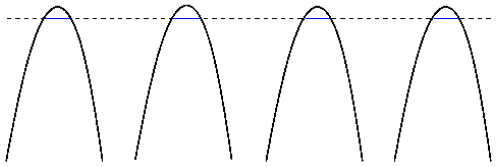
Calculation of scattering matrix for arbitrary potential shape

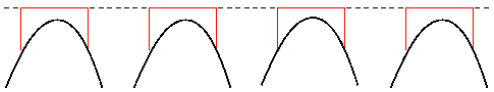


$$(E - H - L)|\Psi_k\rangle = Q|\Psi_k\rangle b_k$$

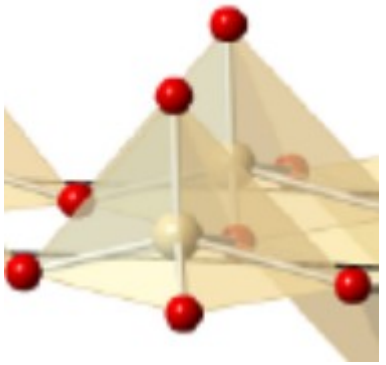
gy, H the hamiltonian,

$$L = \frac{1}{r}\delta(r - r_o)\frac{d}{dr}r \qquad \text{and} \quad Q = \delta(r - r_o)$$

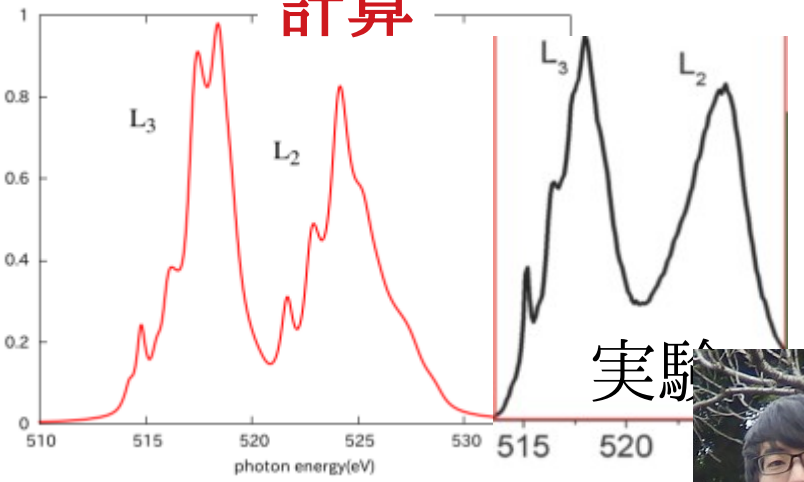




V_2O_5



計算

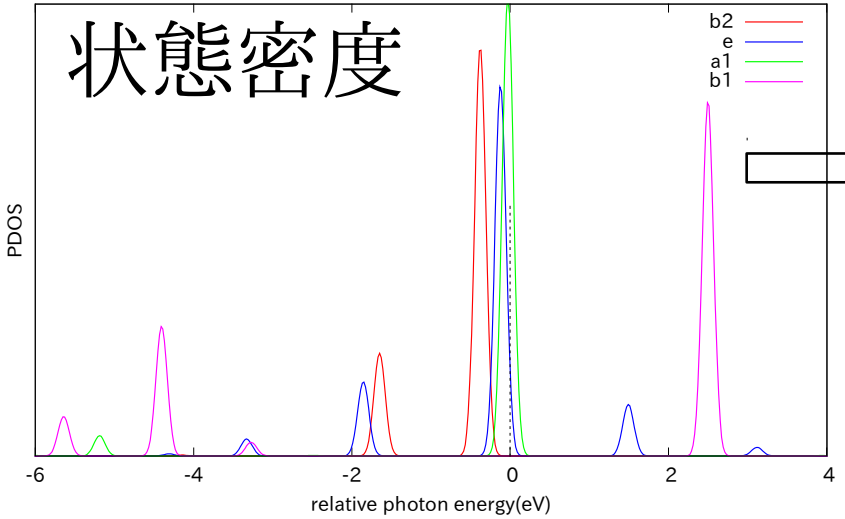


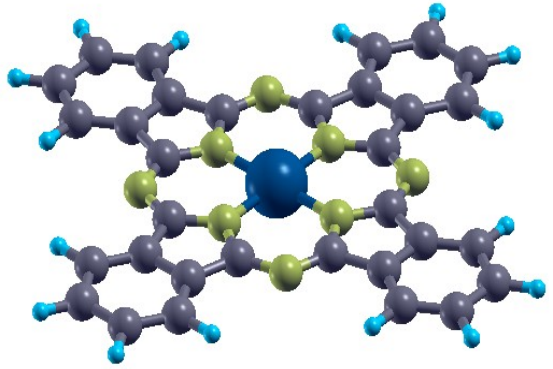
実験

X線吸収理論
経験的なパラメータなしの多重項モデル

DFT

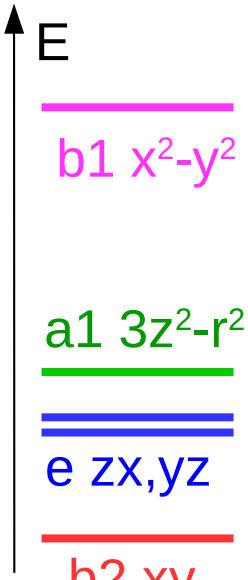
状態密度



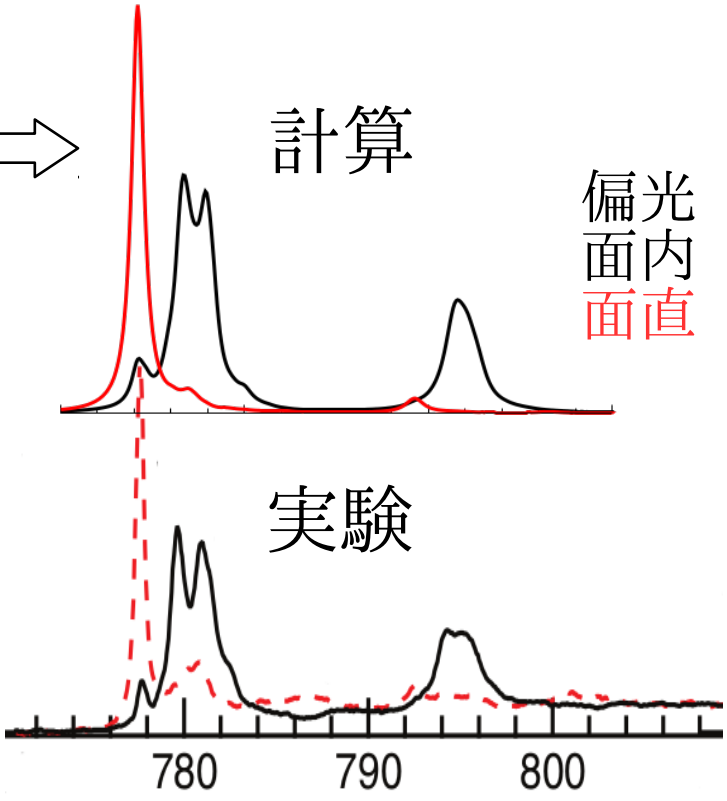


Co-Pc

配位子場



多重項理論



X線エネルギー

D) Theory of finite volume fluctuations in fluids

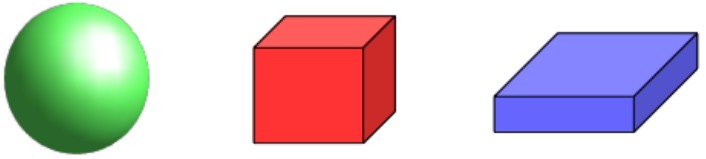
Thermodynamic response functions, e.g. compressibility, relate to particle fluctuations and can be calculated as infinite volume [“Kirkwood-Buff”] integrals over pair correlation function h(r)

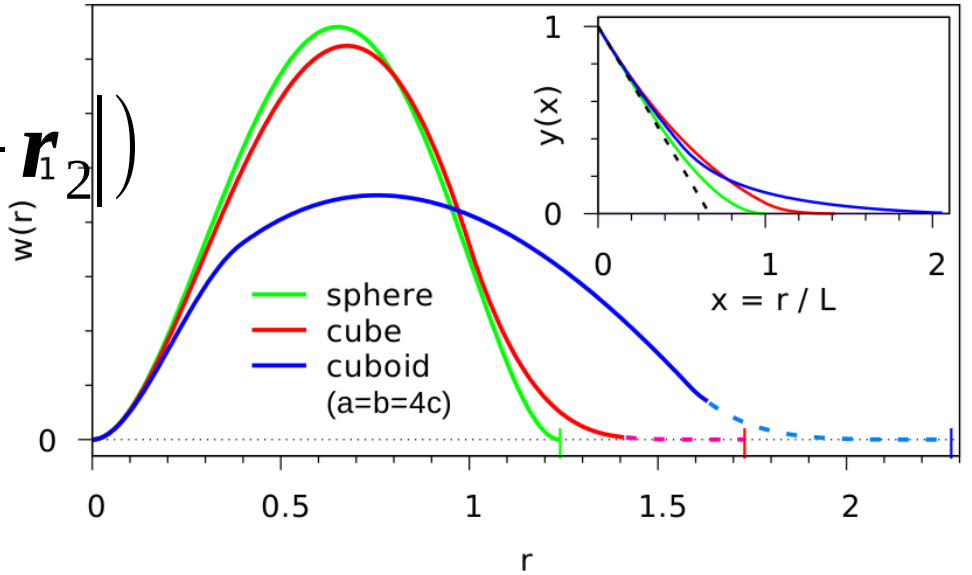
We have generalized Kirkwood-Buff theory to finite volumes and solved the long standing problem of slow integral convergence

$$G(\infty) = \int_0^\infty h(r)\, 4\pi r^2\, dr$$

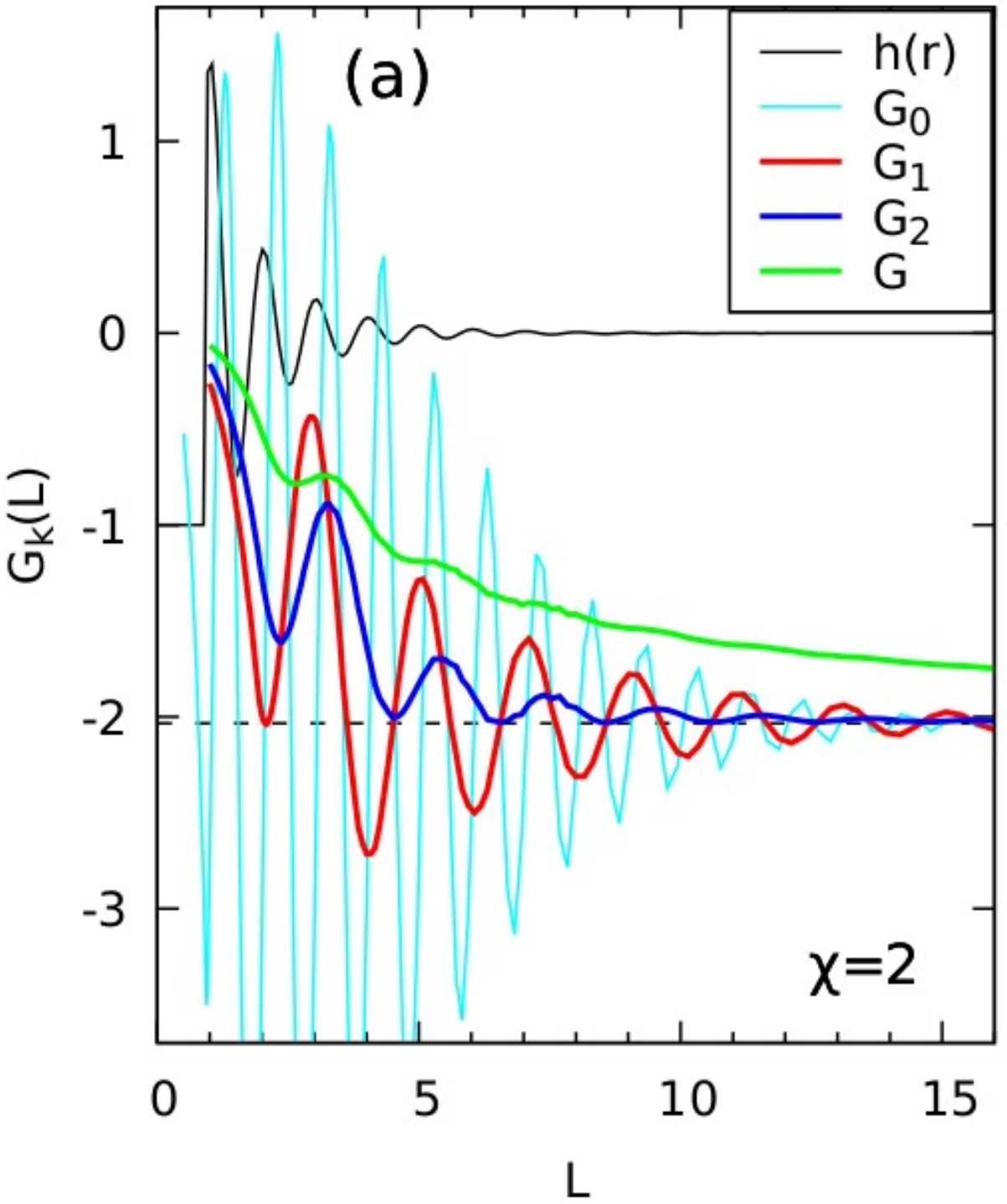
$$G(V) = \int_V d\boldsymbol{r}_1 \int_V d\boldsymbol{r}_2\, h\left(\left|\boldsymbol{r}_1 - \boldsymbol{r}_2\right|\right) = \int_0^L h(r)\, w(r, V)\, dr$$

Analytic weight functions w(r,V)



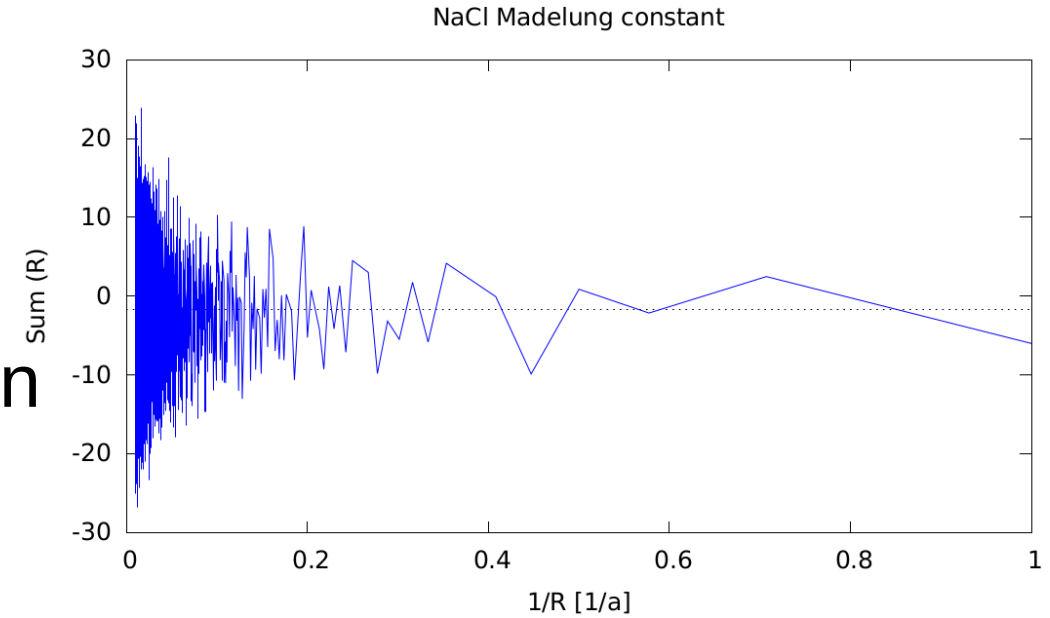


Standard truncated integral (G_0) vs exact finite volume (G) and new extrapolations (G_1,G_2) to ∞



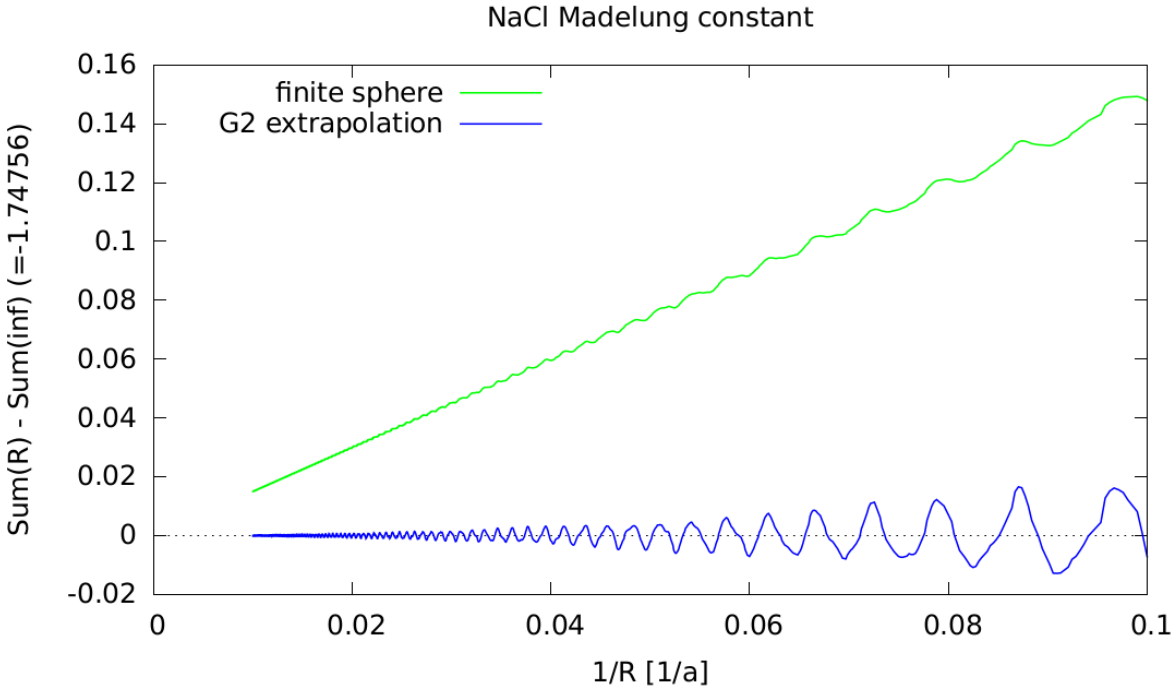
Application to crystals: Madelung constant

spherical shell summation
→ divergence



finite volume
KBI method

→ fast convergence



Thermodynamics of alloys from pair-distribution function / X-ray diffraction data

1) Application of fluctuation theory to finite crystalline nanoparticles of spherical or cubic shape with simple cubic, bcc, or fcc structure

a) generate RDF for perfect crystal

b) apply finite volume Kirkwood-Buff integral theory to compute Gij and compressibility as a function of cluster size

b) compare with liquid and bulk crystal

2) Alloy theory

a) Generate model pair distribution function with Monte Carlo simulation and apply KB theory

b) apply theory to experimental structure factor / PDF

Refs:

P.K. et al. J. Phys. Chem. Letters 4 (2013) 235.

P.K. and T.J.H.Vlugt. Phys Rev. E 97 (2018) 051301