Exercises

- Recommended trials
- Exercises 1-8

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Recommended trials

1. Geometry optimization

   Perform a geometry optimization using ‘Methane2.dat’.
   See the page 65 in the manual.

2. Density of states

   Calculate DOS using ‘Cdia.dat’
   See the page 79 in the manual.

All the input files can be found in the directory ‘work’.

3. Wannier functions

   Calculate Wannier functions for Si bulk using ‘work/wf_example/Si.dat’, and perform the band interpolation. See the page 159 in the manual.

4. Reaction barrier by the nudged elastic band (NEB) method

   Calculate a reaction barrier using ‘C2H4_NEB.dat’.
   See the page 182 in the manual.

5. Transmission of a carbon chain

   Calculate an electric transmission of a carbon chain using ‘Lead-Chain.dat’, ‘NEGF-Chain.dat’. See the page 136 in the manual.

6. Spin-orbit coupling

   Calculate a band structure by taking account of SOC using ‘GaAs.dat’.
   See the page 117 in the manual.

Exercise 1

Confirm that the virial theorem is valid for the formation of bonding of a H_2 molecule. This is also a good playground to check dependency of the result on parameters such as basis set, cutoff energy, and etc.

Virial theorem

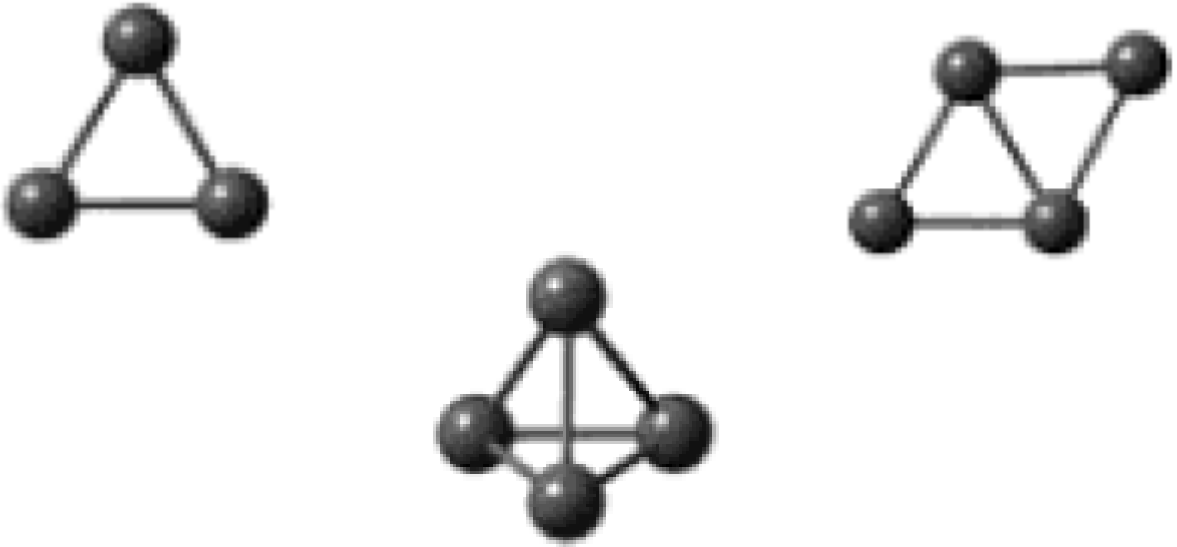
$$2T(R_\infty) + V(R_\infty) = 0$$

$$2T(R_\mathrm{e}) + V(R_\mathrm{e}) = 0$$

$$\begin{aligned} D_\mathrm{e} &= -\left(E(R_\mathrm{e}) - E(R_\infty)\right) \\ &= T(R_\mathrm{e}) - T(R_\infty) \end{aligned}$$

Exercise 2

Try to find stable structures of small Pt clusters using finite temperature molecular dynamics simulations and geometry optimization, and compare your results to the results reported in a paper: L. Xiao, L. Wang, “Structures of Platinum Clusters: Planar or Spherical”, J. Phys. Chem. A 108, 8605 (2004).



Exercise 3

Get familiar with the Effective Screening Medium (ESM) method by reproducing Fig. 45 in the manual of Ver. 3.8.

http://www.openmx-square.org/openmx_man3.8/node138.html
http://www.openmx-square.org/openmx_man3.8/node139.html

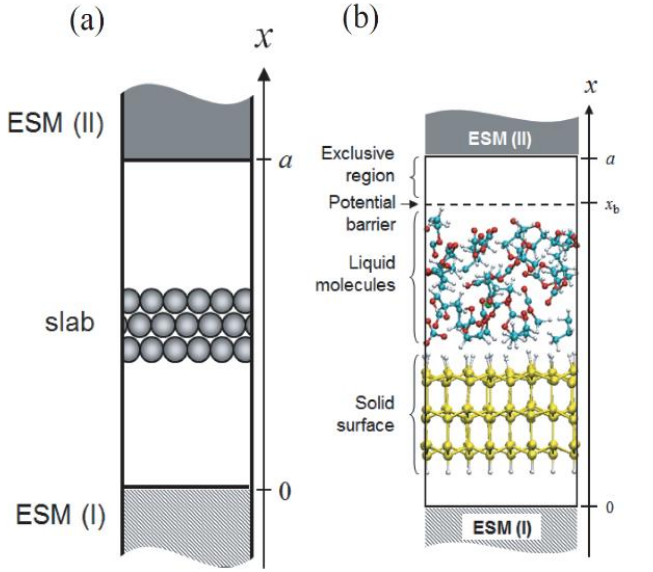


Figure 44: (a) Schematic view of a slab with semi-infinite media (ESMs). ESM (I) and (II) are placed at cell-boundaries, x = 0 and a (a: the length of the cell along x-axis), respectively. (b) An example of a unit cell for a MD calculation of solid surface-liquid interface model system with the ESM method. The slab and ESMs are placed parallel to the y-z plane.

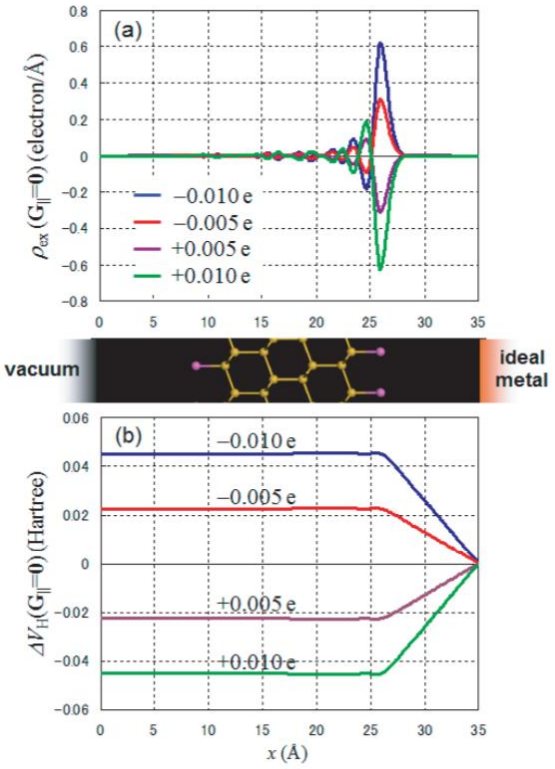
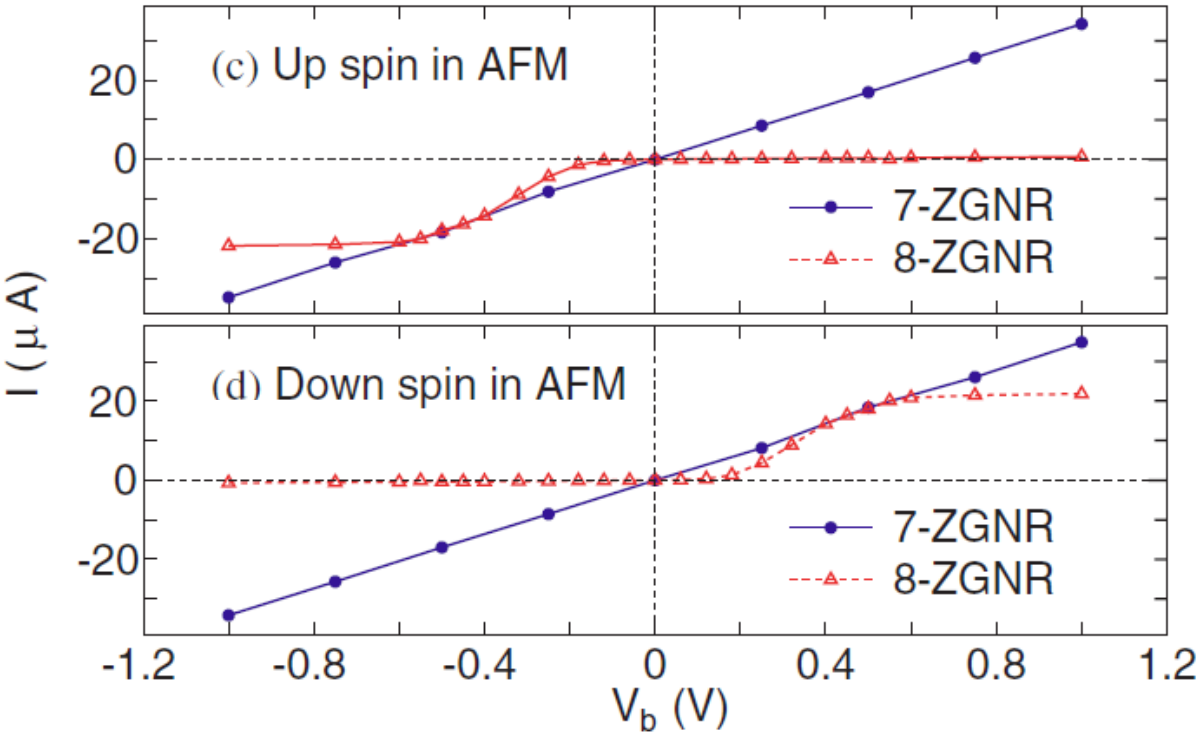
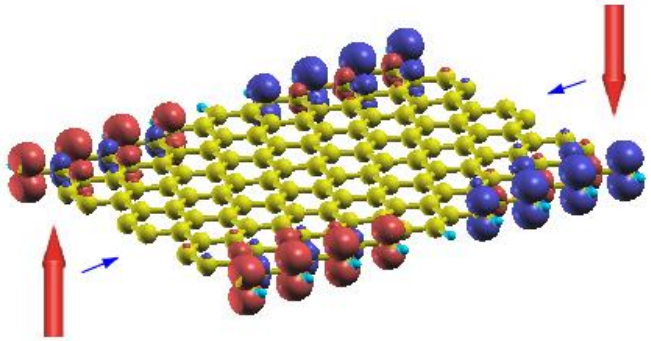


Fig. 45

Exercise 4

Reproduce the dual spin filter effect of 8-zigzag graphene nanoribbon discussed in PRB 81, 075422 (2010).





TO et al., PRB 81, 075422 (2010).

Input files are available in work/negf_example for 8-zigzag graphene nanoribbon with an antiferromagnetic junction under a finite bias voltage of 0.3 V.

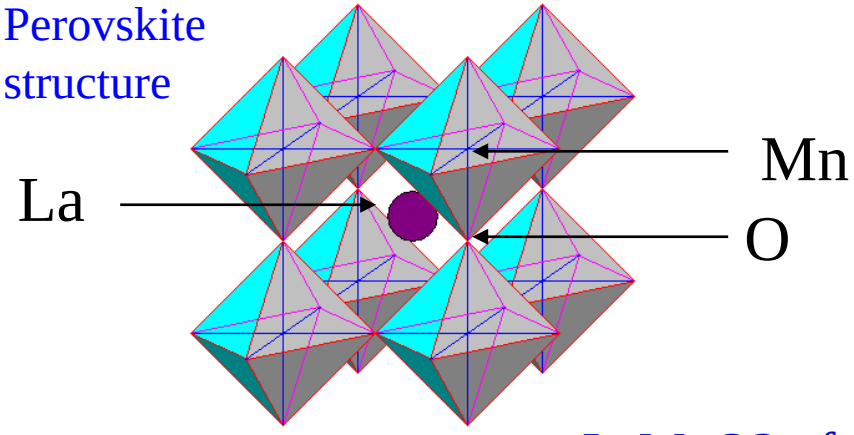
Step 1: Lead-L-8ZGNR.dat, Lead-R-8ZGNR.dat
Step 2: NEGF-8ZGNR-0.3.dat

Exercise 5

Try to calculate total energies of four magnetic structures, FM(ferromagnetic)-type, A-type, C-type AFM(anti-ferromagnetic), of LaMnO3. It is known that the ground state has the A-type AFM structure.

Ref.: Fang et al., PRL 84, 3169 (2000).

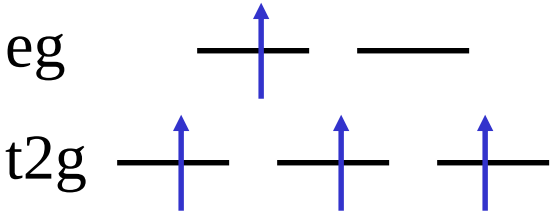
Perovskite structure



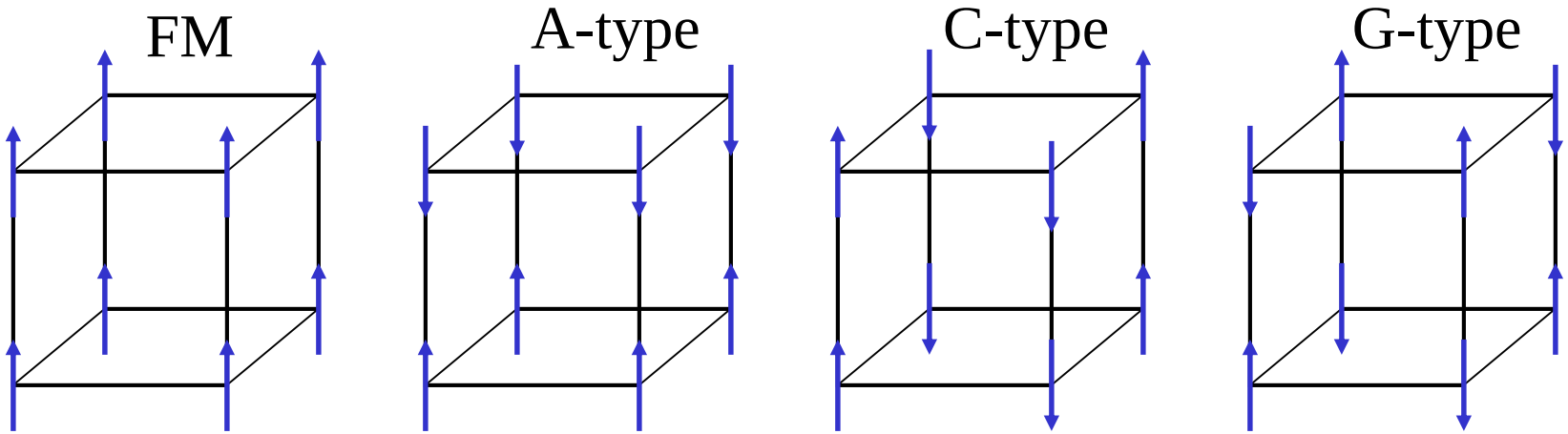
Nominal valence

La^{3+},Mn^{3+}, $O^{2-} \times 3$

Mn^{3+} ($3d^4 4s^0$) in octahedral site



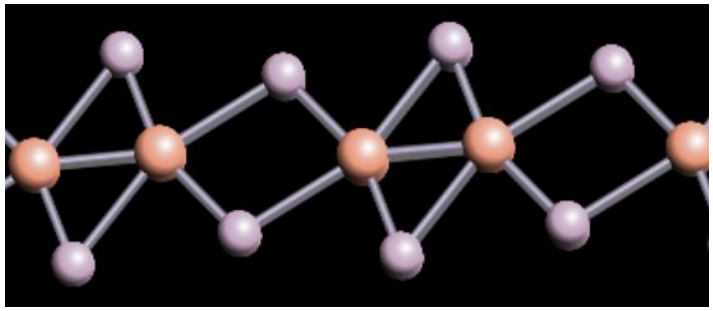
LaMnO3 of magnetic structure



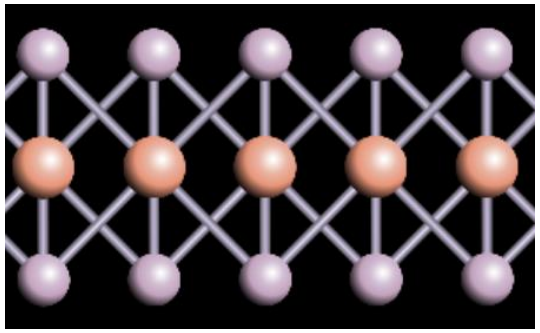
Exercise 6

Perform the variable cell optimization of a single layer of MoA_2 (A=S,Se,Te) in the 1T- and 2H-structures, and compare their total energies and band structures. Discuss a possible electronic structures at the interface structure.
(ref.: W.S. Paz et al., 2D Mater. 4 015014(2017)).

1T

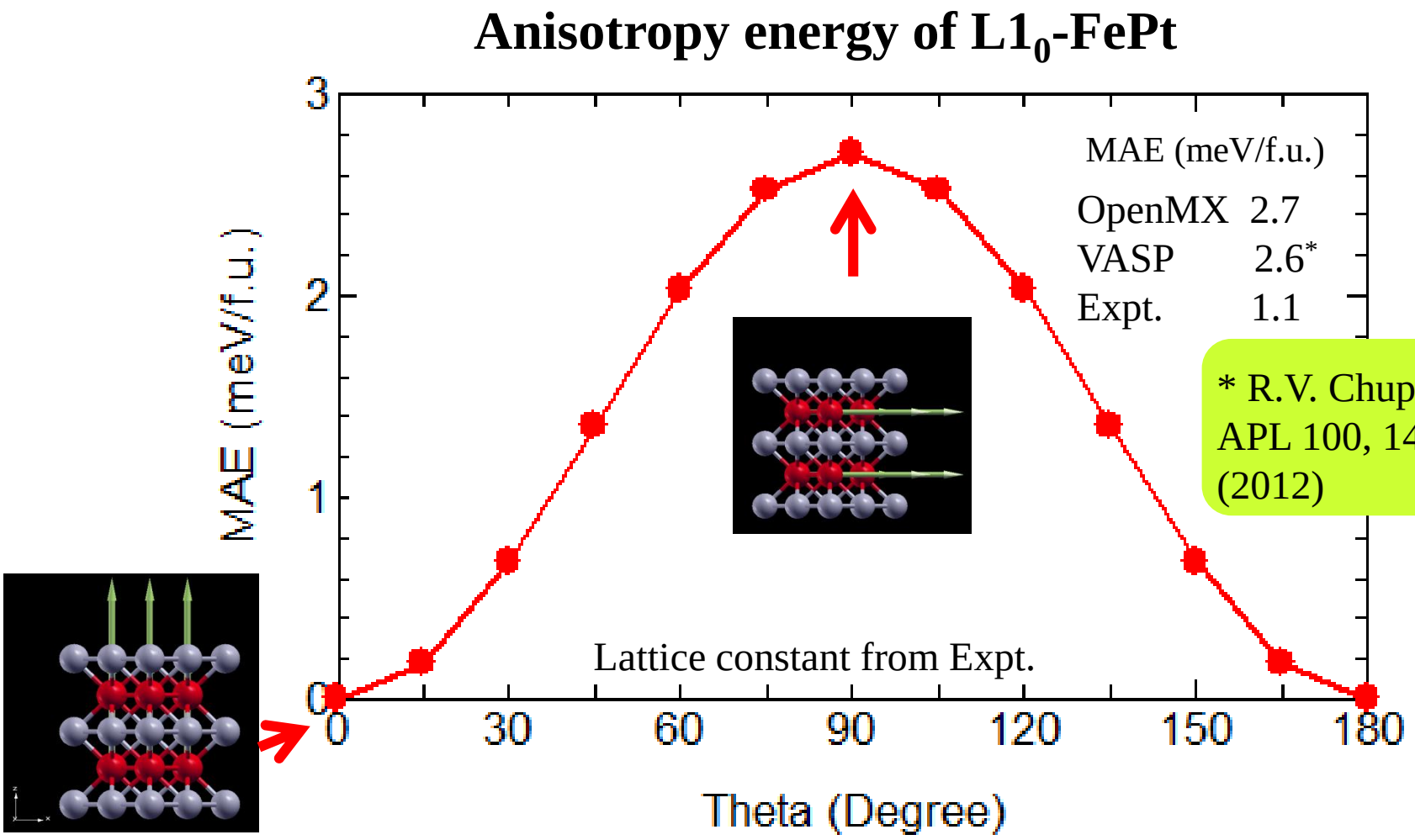


2H



Exercise 7

Calculate a magnetic anisotropy energy of $L1_0$-FePt using the constraint scheme.



Exercise 8

Calculate the absolute binding energy of the C-1s state in TiC.

TABLE I. Calculated binding energy of a core level in bulks.

Material	State	Calculation (eV)	Experiment (eV)
Gapped system			
c-BN	N-1s	398.87	398.1[a]
Bulk NH_3	N-1s	398.92	399.0[b]
Diamond	C-1s	286.50	285.6[c]
Si	Si-2$p_{1/2}$	100.13	99.8[a]
Si	Si-2$p_{3/2}$	99.40	99.2[a]
Semimetal or metal			
Graphene	C-1s	284.23	284.4[c]
TiN	N-1s	396.43	397.1[d]
TiC	C-1s	281.43	281.5[a]

TO and C.-C. Lee, PRL 118, 026401 (2017).

The details can be found in the lecture note for “Core level binding energies in solids from first-principles ”.