Notes of **Computational Material Science**, CHEN Shuang

hebrewsnabla

December 9, 2019

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report: density fitting

score: rescale to 85-98

1 Introduction

1.1 Development

光到电 – SC
电到光 – OLED

memory + resistor = memristor

Two aspects of CMS

1. computational simulation (of real process)
2. computer design

Main Elements of Materials

1. Composition & Structure
2. Synthesis & Processing
3. Properties
4. Performance

MGI, Materials Genome Initiative

DB	founder	institute	
Materials Project	G. Ceder	UCB, MIT	Li battery, zeolites, MOF
AFLOWlib	S. Curtarolo	Duke	
OQMD	C. Wolverton	NW	perovskites, thermoelectrics
NoMaD		马普	
		EPFL	
MatNavi		NIMS	

Table 1

1.2 Methodological System

1.3 Learning

2

Add Valence 加氢
copy: save as .mol – MS

3 Electronic Structure Theory

3.1 HF

3.2 CI

MRCI

3.3 MCSCF, Multiconfiguration Self-Consistent Field

CASSCF, Complete Active Space SCF

3.4 CC

4 QC Computation with Gaussian

Draw MOs
Results – Surfaces
– generate cube

5 Energy Band Theory

5.1

5.2 Reciprocal Space

For a crystal founded by $N_1 \times N_2 \times N_3$ lattices

$$k = \frac{l_1}{N_1} b_1 + \frac{l_2}{N_2} b_2 + \frac{l_3}{N_3} b_3 \tag{5.1}$$

$$R_n G_m = 2\pi N \tag{5.2}$$

Brillouin zone

$$k \cdot G_m = -\frac{1}{2} |G_m|^2 \tag{5.3}$$

PBC SE

$$(\widehat{\mathbf{T}} + \hat{V}(r))\psi_n = E_n \psi_n \tag{5.4}$$

$$V(r) = V(r + R_l) \tag{5.5}$$

Plot $E(\mathbf{k})$ needs 4-D picture, we choose a certain direction to plot 2-D graph.

6 Density Functional Theory

Ab intio 数值基组

6.1

LDA: magnetic
Hybrid: band gap
GGA+U:
GW

7

7.1 E_{cut}

Higher E_{cut}, More accurate. correction factor

$$\frac{\mathrm{d}E_{tot}}{\mathrm{d}\ln E_{cut}} < 0.01\mathrm{eV/atom} \tag{7.1}$$

7.2 Orthogonalized PW, OPW

Herring

7.3 Pseudo-potentials

– NCPP
– USPP

7.4 Tricks

8

9 FPMD

9.1 Introduction

MD:

1. classical
2. semi-classical (tight-binding)
3. FP

Software: CPMD, VASP, CP2K

9.2 BOMD

Hellmann-Feynman force

$$m\ddot{\mathbf{R}}_i = -\frac{\partial E}{\partial \mathbf{R}_i} \tag{9.1}$$

9.3 CPMD

Extended Lagrangian

$$\mathcal{L} = \sum_i^{N_e} \frac{\mu}{2} \int \left|\dot{\psi}_i(\mathbf{r})\right|^2 \mathrm{d}r + \sum_I^{N_{atom}} \frac{M_I}{2} \ddot{\mathbf{R}}_I^2 - E[\{\psi_i\}, \{\mathbf{R}_i\}] + \sum_{ij} \Lambda_{ij} [\int \psi_i^* \psi_j \mathrm{d}r - \delta_{ij}] \tag{9.2}$$

适合 NVE

9.4 Gaussian Plane Waves (GPW) Method

Used by CP2K
GTH pseudo potential

9.5 CP2K Quick Start

Max-Planck -> U of Zurich

9.5.1

Input

- *.inp
-
-

Output

- *.out (summary)
- *.ener
- *.xyz
- *.restart
- *.wfn

9.6 inp

```
&BEGIN section_name [param]
KEYWORD [value]=[...]
 ...
&END section_name
```

- GLOBAL
- EXT_RESTART
- MOTION
- FORCE_EVAL
- DFT
- SUBSYS

```
&GLOBAL
   PRINT_LEVEL          LOW
   PROJECT_NAME         XXX
   RUN_TYPE             MD
&END GLOBAL
```