

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

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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

Table 1

### 1.2 Methodological System

### 1.3 Learning