Thesis Title

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Abstract

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Preface

Chapter 1

Introduction

some introduction on the importance of discovering new materials and alloying.

High-entropy alloys is a novel class of materials based on alloying multiple components, as opposed to the more traditional binary alloys. This results in an unprecedented opportunity for discovery of new materials with a superior degree of tuning for specific properties and applications. Recent research on high-entropy alloys have resulted in materials with exceedingly strong mechanical properties such as strength, corrosion and temperature resistance, etc **find references**. Meanwhile, the functional properties of high-entropy alloys is vastly unexplored. In this study, we attempt to broaden the knowledge of this field, the precise formulation of this thesis would be an exploration on the possibilities of semiconducting high-entropy alloys.

A key motivation of this thesis is the ability to perform such a broad study of complex materials in light of the advances in material informatics and computational methods. In this project, we will employ Ab initio methods backed by density functional theory on top-of the line supercomputers and software. 20 years ago, at the breaking point of these methods, this study would have been significantly narrower and less detailed firstly, but secondly would have totaled ... amount of CPU hours to complete (**Calculate this number**). In the addition to the development in computational power, is also the progress of modeling materials, specifically we will apply a method called Special Quasi-random Structures (SQS) to model high-entropy alloys or generally computationally complex structures. Together with the open landscape of high-entropy alloys described above, these factors produce a relevant study in the direction of applying modern computational methods to progress the research of a novel material class and indicate promising directions within the field.

In specifics, this thesis revolve around the electrical properties of high-entropy alloys, mainly the band gap as this is the key indicator for a semiconducting material and it's applicability. Semiconductors are the building blocks in many different applications in today's world, ranging from optical and electrical devices, to renewable energy sources such as

solar and thermoelectricity. Given the economic and sustainable factors concerning silicon, in addition to its role in relevant applications such as microelectronics and solar power. Silicon emerges as a natural selection to build our alloys around. Furthermore, the development and research on both high entropy alloys and metal silcides have been heavily centered around 3d transition metals. Keeping in line with the economic and environmental factors, we will continue this direction by focusing on high entropy stabilized sustainable and economic 3d metal silicides **Not happy with this writing**. Throughout the study we will analyze a great number of permutations of 3d silicides, from different initial metal silicides such as $CrSi_2$, $FeSi_2$, $MnSi_{1.75}$, Fe_2Si, each with distinct properties relating to the band gap, crystal structure and metal to silicon ratio. In addition, the permutations include numerous metal distributions and elements within the 3d-group of metals. Examples are Co, Cr, Fe, Mn, and Ni.

Given a background in high-entropy alloys, one could ask if this study is truly sensible. In the later sections we will cover the details of this field, and it quickly become clear that the materials investigated in this study does not fall under the precise definition of high-entropy alloys, nor do we intend to explore the properties and factors relating to high-entropy stabilized alloys such as the configurational entropy, phase stability and finite temperature studies. However this study is motivated from the discovery of these materials and promising properties, and venture into a more hypothetical space of materials, enabled by the computational methods available to study the potential properties of such materials. On the other hand, very recent studies **Mari, and other HEA silicide study** have experimentally produced high-entropy disilicides, thus in some way justifying the direction of this project.

We begin this project by reviewing key concepts of solid-state physics for readers lacking a background in materials science, and an introduction to the base 3d silicides of the experimental work. Later follows a theoretic walk-through of the relevant concepts of this thesis, these topics include high-entropy alloys, special quasi-random structures, and density functional theory. Next we shine light on the implementation of DFT in this project, and other computational details required to reproduce the results in this thesis, such as the use of the Vienna Ab Initio Simulation Package (VASP) and implementation of SQS. Finally we present the results of our study, these include the band gap and electronic properties of various structures and the success and challenges of the computational methods applied throughout the study.

Part I

Theory

Part II

Methodology and Implementation

mm

Part III

Results and Discussion

Chapter 8

Working title

In the introduction to this project, we briefly discussed the scope and focus of the thesis. In figure/table .. we have displayed the complete list of structures, compositions and permutations of high-entropy silicides trialed throughout the duration of the project. **Make figure.** Amidst the large number of structures, we found particularly promising attributes of $(CrFeMnNi)Si_2$ (CFMN) SQSs based on the orthorombic crystal structure of $FeSi_2$, thus we will begin this section by presenting the results regarding this structure.

In this structure, each supercell consist of 48 total atoms, 32 of which is silicon, and the remaining 16 positions is equally distributed between Chromium, iron, manganese, and Nickel. The 5 distinct SQS supercells can be seen in figure (method/SQS). In table **??** we present a summary of the most relevant functional properties of the SQSs.

Structure	Total energy/atom (eV)	Final magnetic moment (?)	Band gap (eV)
A	-6,6080	4.0006	0.0280
B	-6,6138	3.9999	0.0523
C	-6,6063	4.0008	0.0344
D	-6,6155	4.0001	0
E	-6,6089	4.0000	0.0495

Table 8.1: Total energy per atom, final magnetic moment, and band gap (GGA) of 5 $Cr_4Fe_4Mn_4Ni_4Si_{32}$ SQSs based on $FeSi_2$

Bellow we have plotted the total density of states corresponding to the five distinct SQSs.

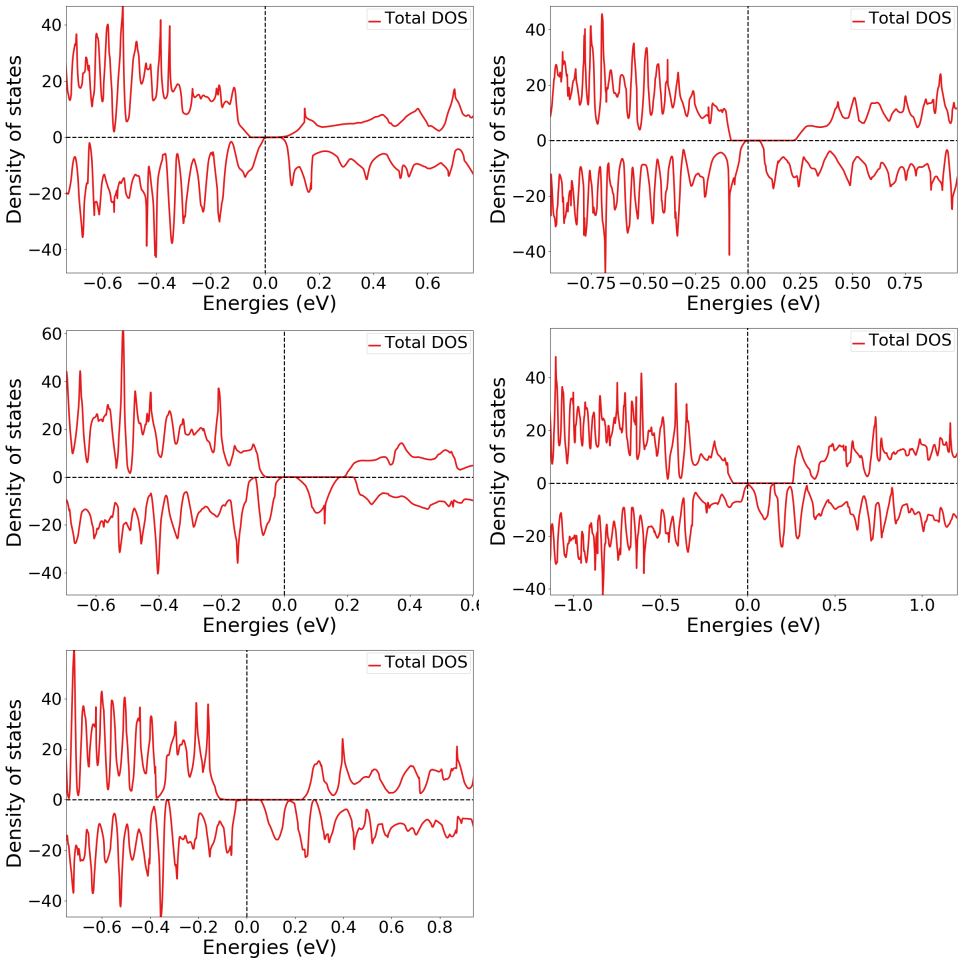


Figure 8.1: Density of states for structure A, B, C, D, E of $CFMNSi_2(FeSi_2)$ SQSs (PBE GGA)

Structure	Spin-up	Spin-down	Total
A	0.0814	0.0522	0.0281
B	0.2932	0.0523	0.0523
C	0.2355	0.0343	0.0343
D	0.3386	0	0
E	0.3078	0.0495	0.0495

Table 8.2: Band gap (GGA) in spin up and spin down channels of CFMNSi2 structures

Structure	PBE	SCAN	HSE06
A	0.0281	0.0000	0.0207
B	0.0523	0.0890	0.1808
C	0.0344	0.0690	0.0196
D	0.0000	0.0000	0.0000
E	0.0495	0.1048	0.0133

Table 8.3: Band gap of $CFMN(FeSi_2)$ SQSs with GGA (PBE), meta-GGA (SCAN) and hybrid-functionals (HSE06). **Add footnote to explain the uncertainty in these results regarding smearing type and width, and DOS and EIGENVAL**

Looking at the results from different functionals, we observe that the hybrid functional HSE06 more or less agree with results of the PBE functional in terms of the actual presence of the band gap, while the size of the gap is up for debate. Especially in B, where we observe a band gap greater than 0.18 eV in comparison to 0.05 eV with PBE and 0.08 with SCAN. Bellow we show the total density of states around the fermi energi E_f for this structure with the HSE06 functional.

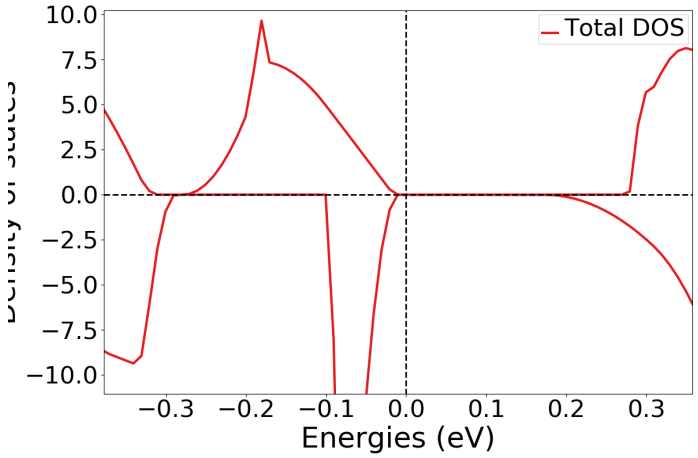
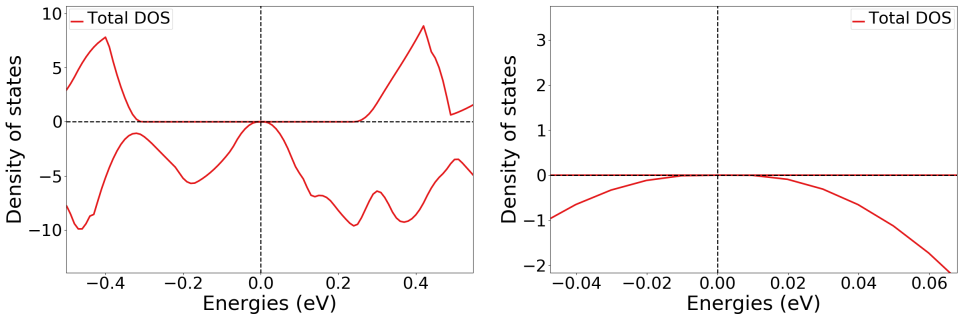


Figure 8.2: Density of states from HSE06 of $FeSi_2$ CFMN structure B

If we now compare this to the density of states of structure E,



(a) DOS ↑, ↓ (b) DOS ↓

Figure 8.3: The density of states of CFMN ($FeSi_2$) structure E for a) spin up and down, and b) focused on spin down

it's obvious that the wider band gap of structure B stems from the spin down channel, as opposed to the other structure where we observe large gaps in ↑ and small nonzero gaps in ↓ except for D with metallic characteristic in spin ↓.

Part IV

Conclusion