



Ab initio study of the electronic structure of orthorhombic iron selenide

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INTRODUCTION

Iron selenide (FeSe) is a key subject of research among iron-based superconductors due to its structural simplicity and the rich interplay between nematicity, magnetism, and superconductivity. Upon cooling below 70–100 K, stoichiometric FeSe undergoes a structural transition from a tetragonal phase to an orthorhombic phase, which is associated with nematic electronic order.

Here we present the relatively understudied band structure and magnetic moments of low-temperature phase calculated using DFT method.

METHODOLOGY

Full-potential linearized augmented plane wave (FP-LAPW) calculations:

- GGA PBE correlation potential
- Elk code implementation

RESULTS

The study analyzed site-projected magnetic moments at the Fe and Se sites, decomposed into spin and orbital contributions. A pronounced **magnetic anisotropy** was revealed: the total magnetic moment along the *c*-axis is approximately three times larger than the moment along the *a*-axis. This effect is governed by a delicate balance between spin and orbital (Van Vleck) moments on the iron sublattice, while the selenium sublattice carries an antiferromagnetically coupled induced moment

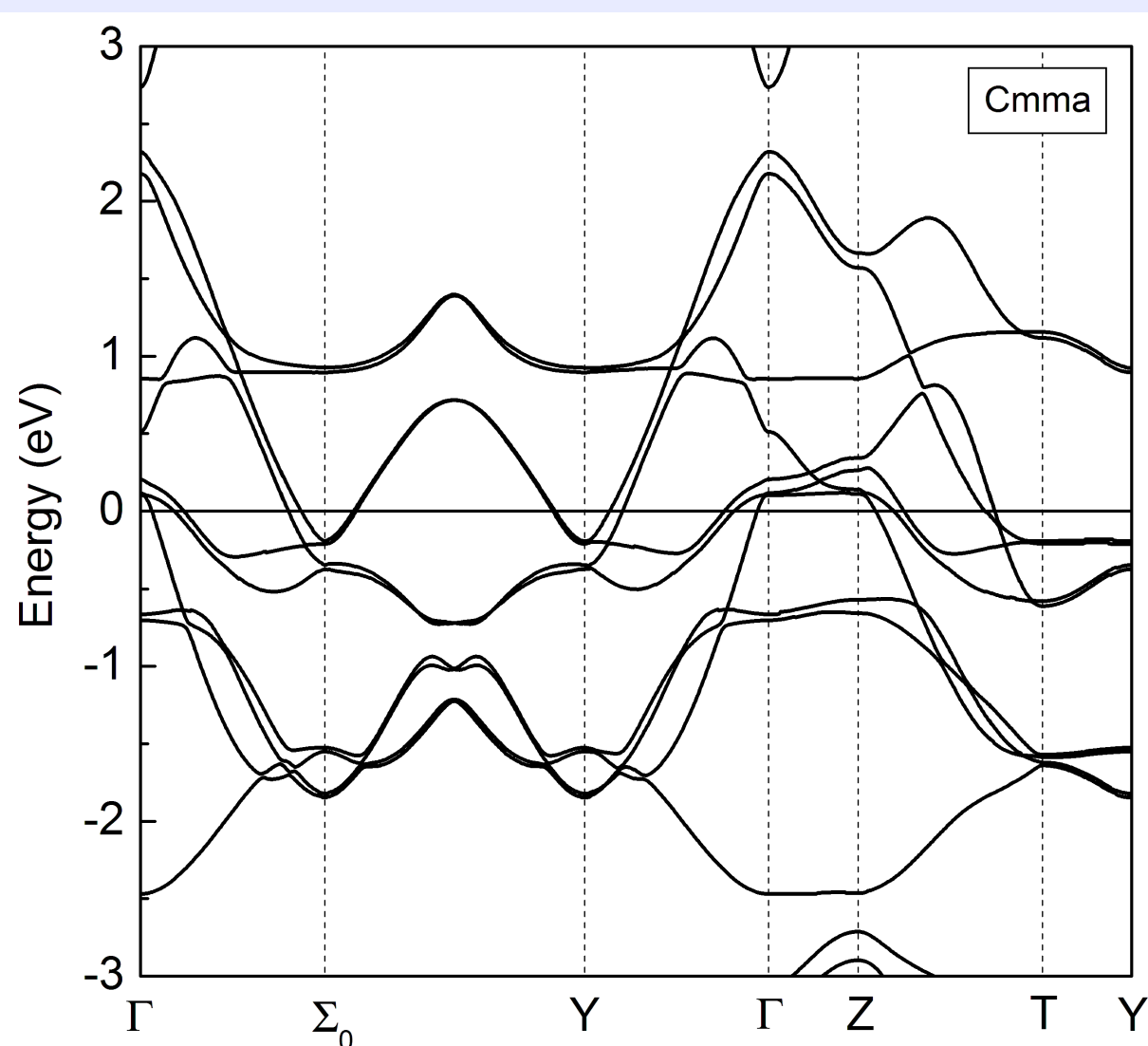


Figure 1: Band structure for FeSe in orthorhombic (*Cmma*) phase

Table 1. Spin, orbital, and total magnetic moments on iron and selenium atoms induced by field $H=10$ T

			H a	H b	H c	J_c/J_a	J_c/J_b	$\langle J \rangle$
P=0 GPa	Fe	L	-2,054556	-2,044724	-1,218287			
	Fe	S	2,479659	2,453185	2,477597			
	Fe	J	0,425102	0,408461	1,259311	2,962	3,083	0,697625
	Se	L	-0,111625	-0,111899	-0,134548			
	Se	S	-0,191616	-0,193666	-0,197767			
	Se	J	-0,303241	-0,305565	-0,332315	1,096	1,088	
	Fe+Se	L+L	-2,166181	-2,156623	-1,352835			-1,89188
	Fe+Se	S+S	2,288043	2,259520	2,279830			2,27580
	Fe+Se	J+J	0,121862	0,102896	0,926995	7,607	9,009	0,38392

			H a	H b	H c	J_c/J_a	J_c/J_b	$\langle J \rangle$
P=0.25 GPa	Fe	L	-1,979329	-1,979022	-1,186083			
	Fe	S	2,787438	2,745613	2,740890			
	Fe	J	0,808109	0,766590	1,554807	1,924	2,028	1,043169
	Se	L	-0,111599	-0,111554	-0,133652			
	Se	S	-0,215047	-0,214733	-0,214759			
	Se	J	-0,326646	-0,326287	-0,348411	1,067	1,068	
	Fe+Se	L+L	-2,090927	-2,090576	-1,319735			-1,83375
	Fe+Se	S+S	2,572391	2,530879	2,526132			2,543134
	Fe+Se	J+J	0,481463	0,440303	1,206397	2,506	2,740	0,709388

SUMMARY

Calculations performed for a modest applied pressure (0.25 GPa) demonstrate that even a small compression of the lattice leads to a marked **enhancement of the total moment on iron**. The primary driver for this is a breakdown of spin-orbital compensation: the spin moment increases while the orbital contribution is partially suppressed. These theoretical results are qualitatively consistent with available experimental data regarding the increase of the magnetic response in the *Cmma* phase