Ab initio Study of the Electronic Structure of Orthorhombic Iron Selenide

Authors A.A. Lyogenkaya, A.S. Panfilov, I.P. Kobzar, A.V. Logosha, G.E. Grechnev, A.V. Fedorchenko
e-mail: lyogenkaya@ilt.kharkov.ua

Affiliations B.Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, Kharkiv, Ukraine

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 electronic band structure and magnetic moments of the low-temperature orthorhombic phase calculated within density functional theory (DFT).

METHODOLOGY

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

- GGA-PBE exchange-correlation functional
- Elk code implementation

RESULTS

We analyzed site-projected magnetic moments at the Fe and Se sites, decomposing them into spin and orbital contributions. A pronounced magnetic anisotropy was found: 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 induced moment antiferromagnetically coupled to the iron sublattice

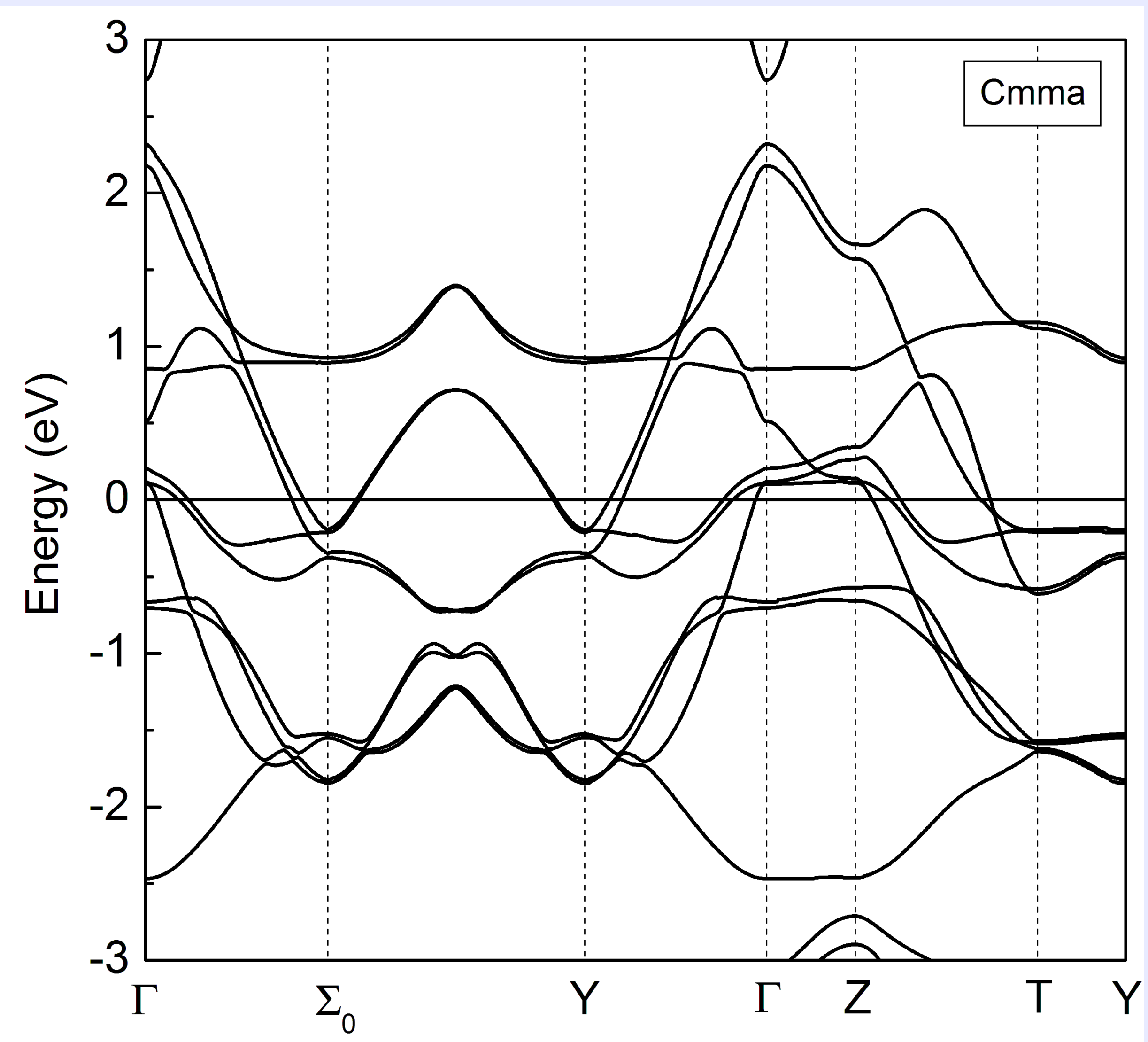

Figure 1: Electronic band structure of FeSe in the orthorhombic Cmma phase

Table 1. Spin, orbital, and total magnetic moments induced on Fe and Se atoms by an external magnetic field of H = 10 T

			H‖a	H‖b	H‖c	J_c/J_a	J_c/J_b	<J>
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	<J>
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 origin of this effect is the reduced compensation between spin and orbital contributions: the spin moment increases while the orbital contribution is partially suppressed. These theoretical results are qualitatively consistent with available experimental observations of the enhanced magnetic response of the Cmma phase under pressure.