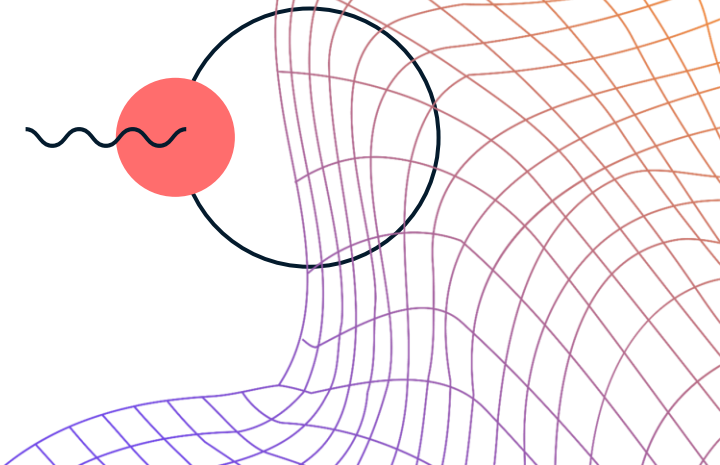
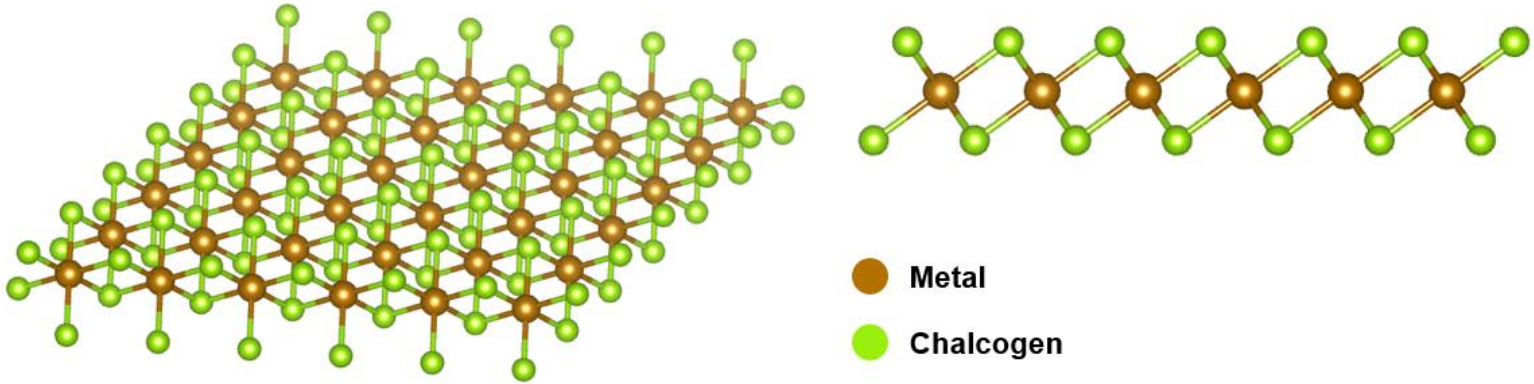
First principles study of Janus Monolayer Transition Metal Dichalcogenides with a substitutional doping



Reynaldo Jauregui

INTRODUCTION

TMDs are represented by the formula **MX2**, where **M** represents a transition metal and **X** a chalcogen atom such as S, Se, or Te. Their structure consists of a layer of the transition metal sandwiched between two layers of chalcogens, joined by covalent bonds.



RELEVANCE OF THE RESEATCH

Iron is a classical magnetic element, which can form 2D magnetic transition metal dichalcogenides (FeX_2), which promising application in spintronic. The family of iron dichalcogenides is mainly composed of three members, FeS_2, $FeTe_2$ and $FeSe_2$, the latter being the least studied of this group of materials.

PURPOSE

The purpose of this work is to study the effect of substitutional doping on the electronic and magnetic properties of the FeSe2 monolayer through first-principles calculations.

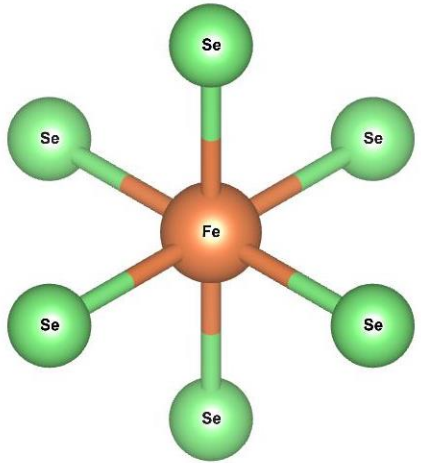
COMPUTATIONAL DETAIL

Exchange-correlation functional	GGA
Kinetic energy cutoff	350 eV
Energy convergence criterion	$1x10^{-6}$ eV
Forces convergence criterion	$1x10^{-5}$ eV/Å
Unit-cell k-mesh size	6x6x1
Supercell k-mesh size	4x4x1
Vacuum	22 Å

RESULTS

ESTRUCTURAL RELAXATION

The structural relaxation was performed to optimize the atomic positions and lattice parameters of the material to find its most stable configuration with the lowest total energy. analysis of the lattice parameters and the bond length was performed to compare the changes on the monolayer unit-cell structure before and after the relaxation process.



$FeSe_2$ Structure	a (Å)	b (Å)	c (Å)	Fe-Se bond length (Å)
Unit-cell	3.20213	3.20213	22.00000	2.28296
Relaxed unit-cell	3.44702	3.44702	19.60614	2.56381

ESTRUCTURAL RELAXATION

Research	Lattice parameter (Å)
1	3.250
2	3.430

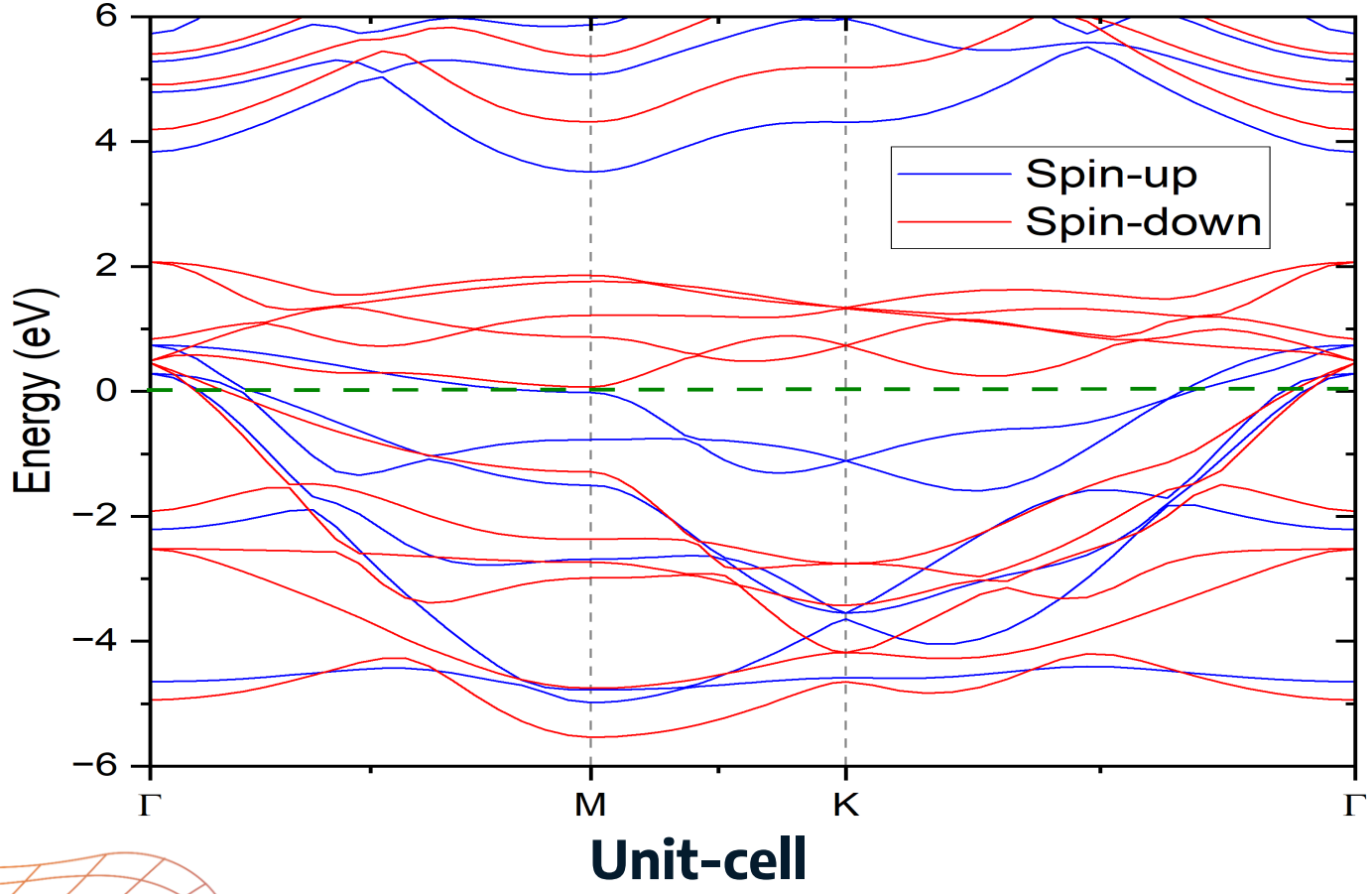
$FeSe_2$ Structure	a (Å)	b (Å)	c (Å)	Fe-Se bond length (Å)
Supercell	6.40426	6.40426	22.00000	2.28296
Relaxed supercell	6.92219	6.92219	19.44695	2.55665

$FeSe_2$ Structure	a (Å)	b (Å)	c (Å)	Fe-Se bond length (Å)	Fe-Co bond length (Å)
Supercell	7.40328	7.40328	22.00000	2.54459	2.63638
Relaxed supercell	7.40991	7.40991	16.97124	2.54548	2.64059

MAGNETISM

Structure	Total magnetic moment (μB)
Unit-cell	4.077
Supercell	15.911
Co-doped supercell	18.619

ELECTRONIC BAND STRUCTURE



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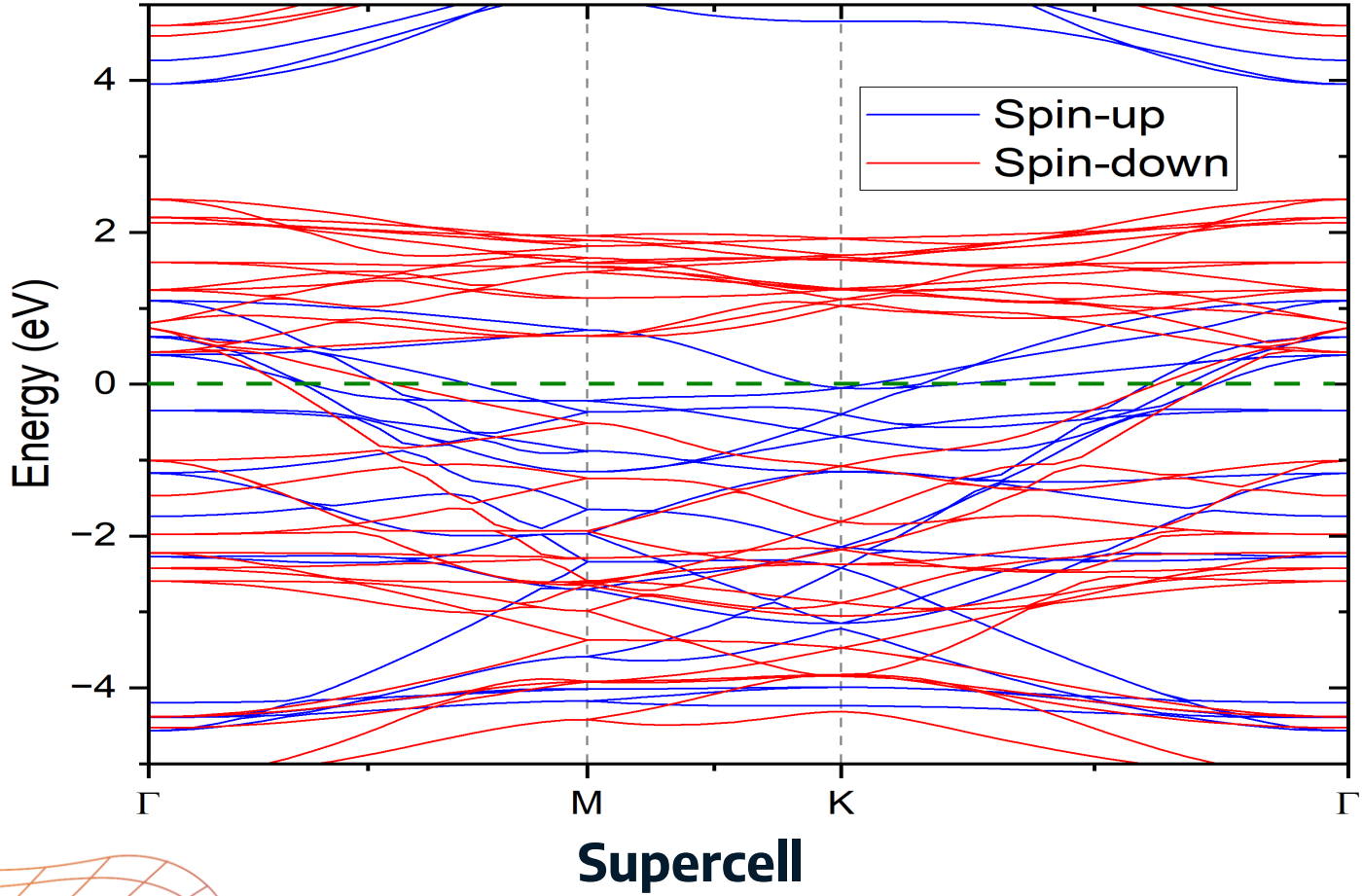
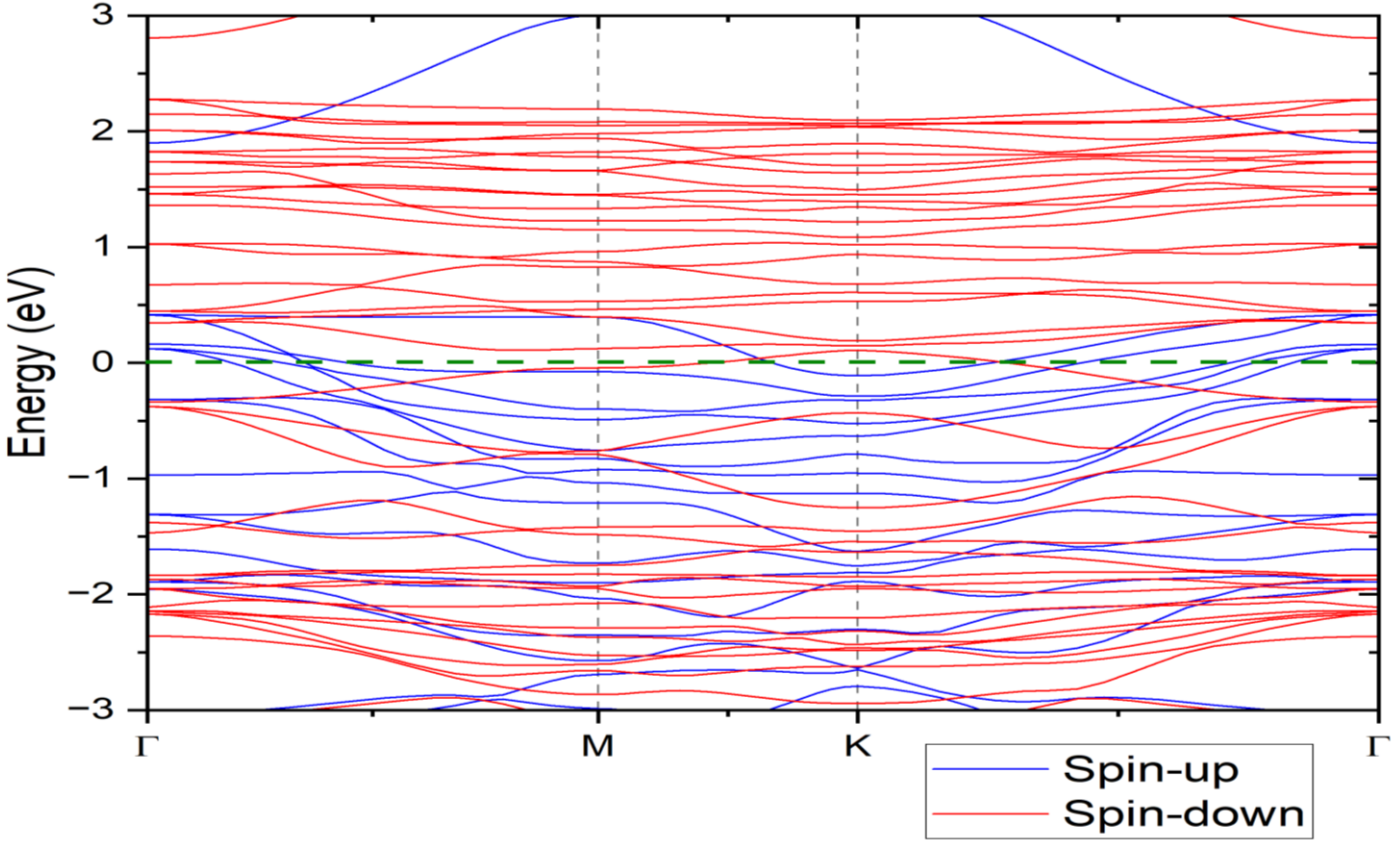
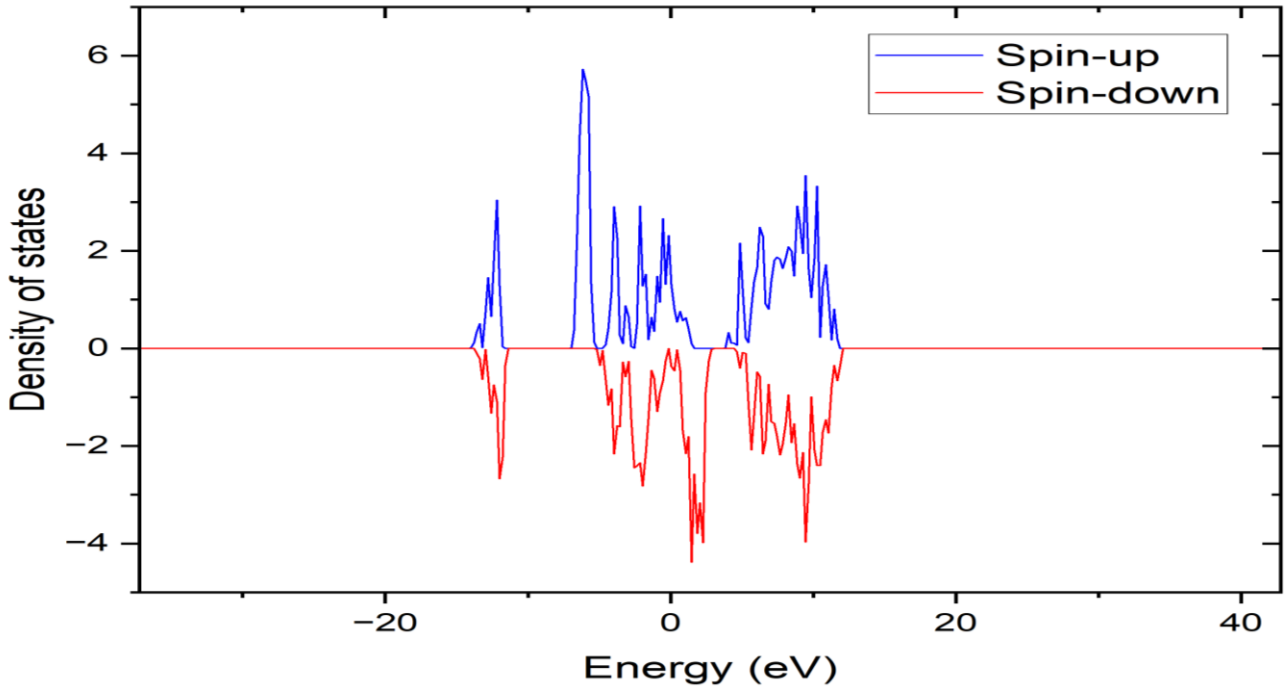


ELECTRONIC BAND STRUCTURE



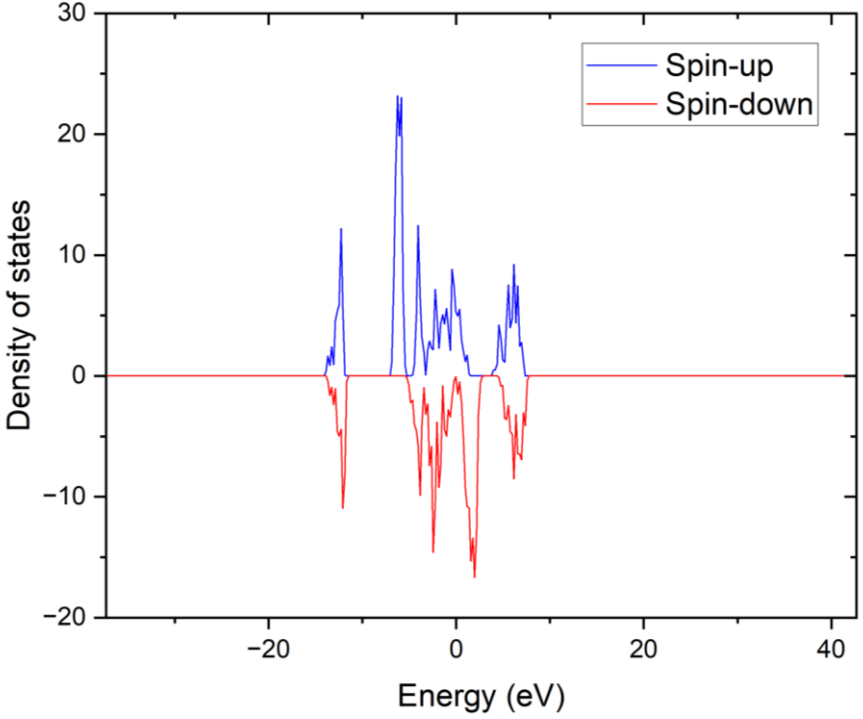
Co-doped supercell

DENSITY OF STATES (DOS)

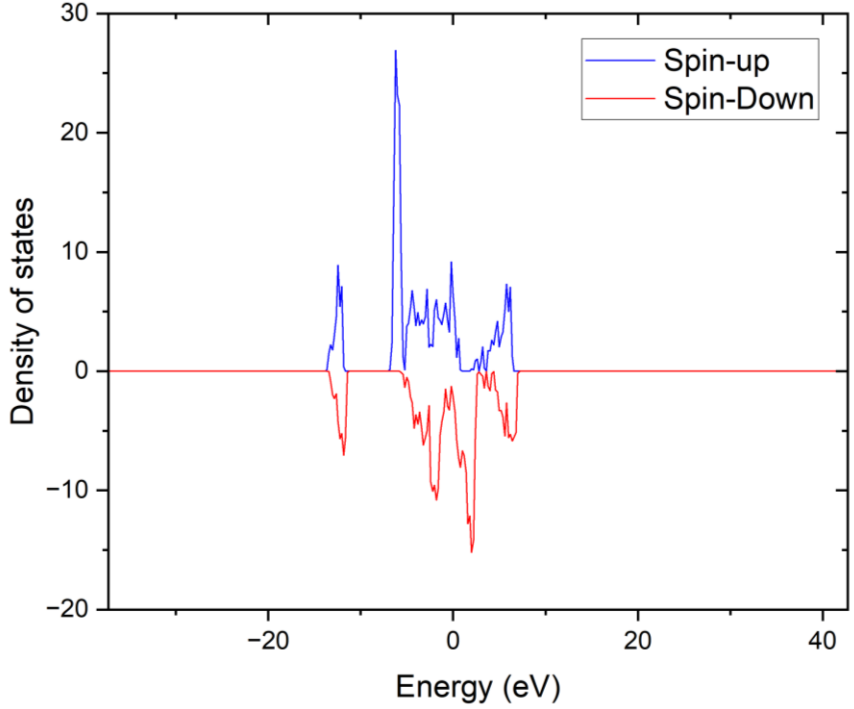


Unit-cell

DENSITY OF STATES (DOS)

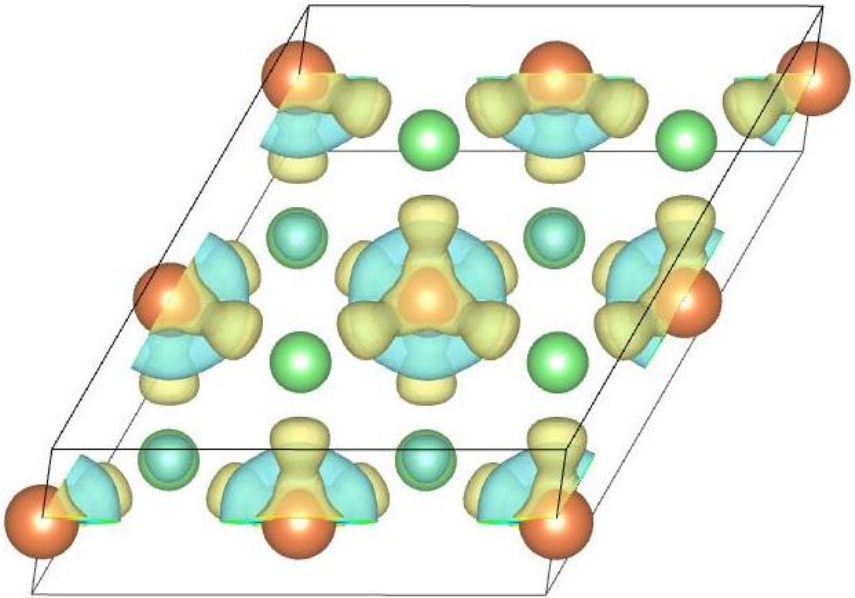


Supercell

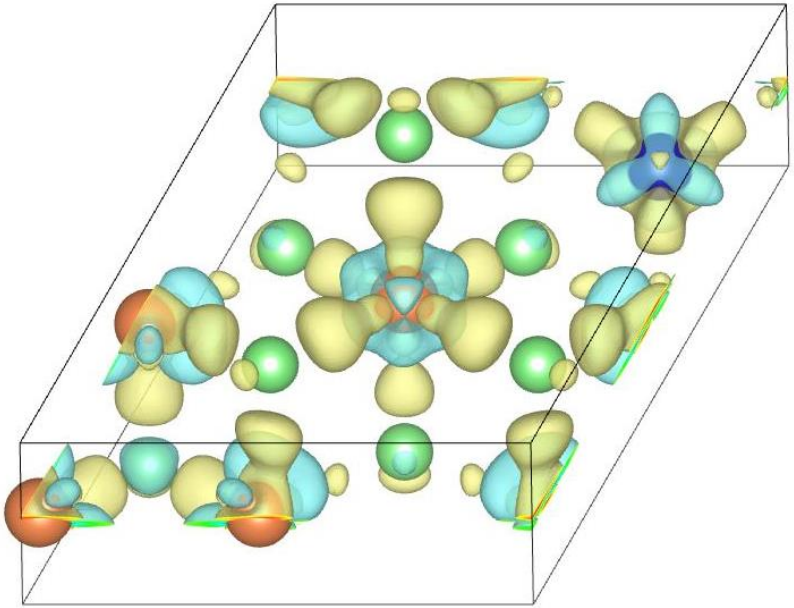


Co-doped supercell

CHARGE DENSITY



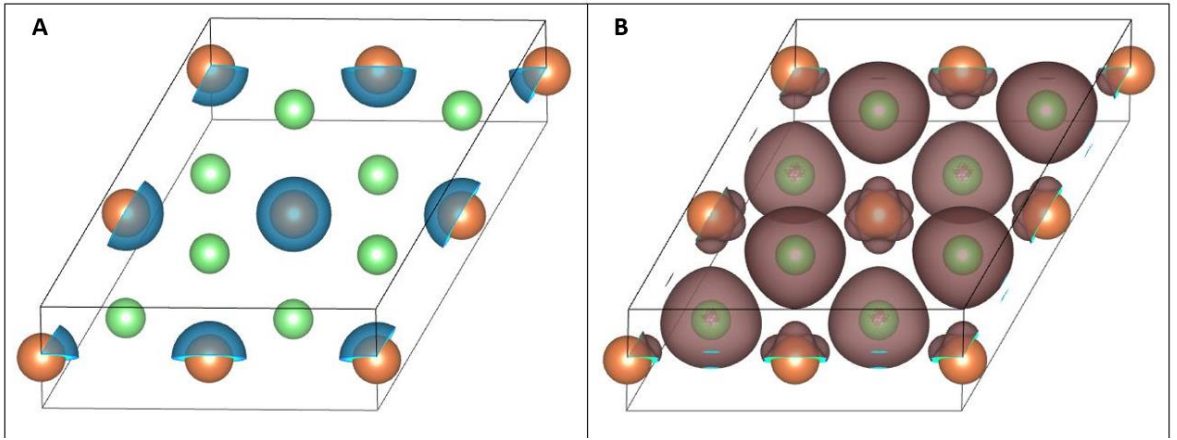
Supercell



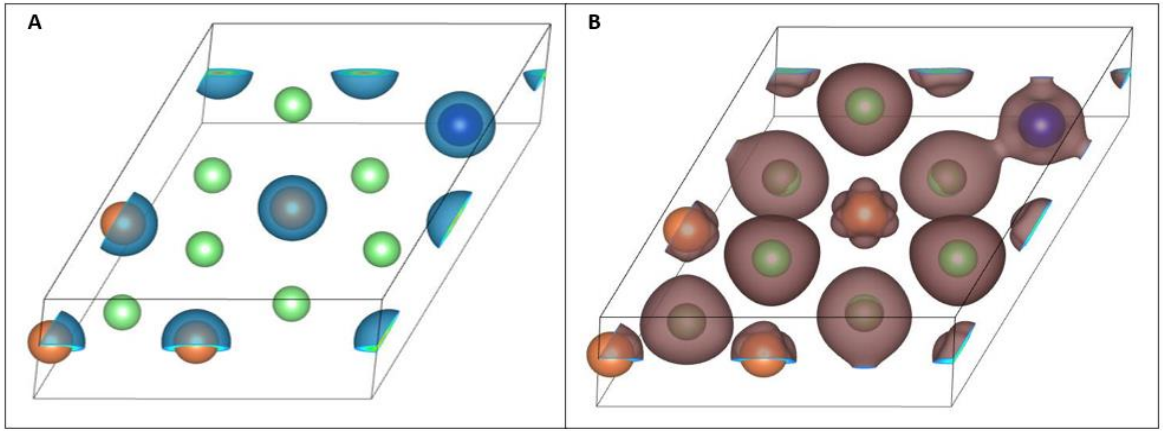
Co-doped supercell

CHARGE DENSITY

Supercell



Co-doped supercell



CONCLUSIONS

1. The structural relaxation of the FeSe2 monolayer generate an increase in the Fe-Se covalent bond length, and therefore the lattice parameter in both unit-cell and supercell structures, due to the new atomic position of the Fe and Se atoms after the relaxation process. On the other hand, the addition of Co into the supercell structure leads to changes in the bond length, decreasing the distance in the Fe-Se bond, while increase the distance of the Fe-Co bond in the relaxed structure.

2. The electronic band structure analysis shows that the FeSe2 monolayer unit-cell have a metallic behavior, since the spin-up and spin-down bands cross the Fermi level. The supercell showed an increase in the number of electronic states for both spin-up and spin-down electrons, when it is compared with de band structure of the unit-cell. Furthermore, the substitution of a chalcogen atom by Co increase the electronic states available in the structure.

CONCLUSIONS

3. The introduction of Co in the structure leads to an increment of electronic states in the supercell.

4. The study confirms the magnetic behavior of the FeSe2 monolayer and demonstrate the effect of the Co on the total magnetic moment, leading to a significant increment in magnetism.

5. The study of the charge density distribution showed that the present of Co in the structure, produced changes in the spatial distribution of charge, leading to changes in the charge accumulation and depletion zones.

6. The substitutional doping with Co proved to be an effective method to change the spin density of the structure.


THANK YOU!