Correlation between of chemical environment and ferromagnetism in the Fe-doped and Zn-vacancy defected ZnSe

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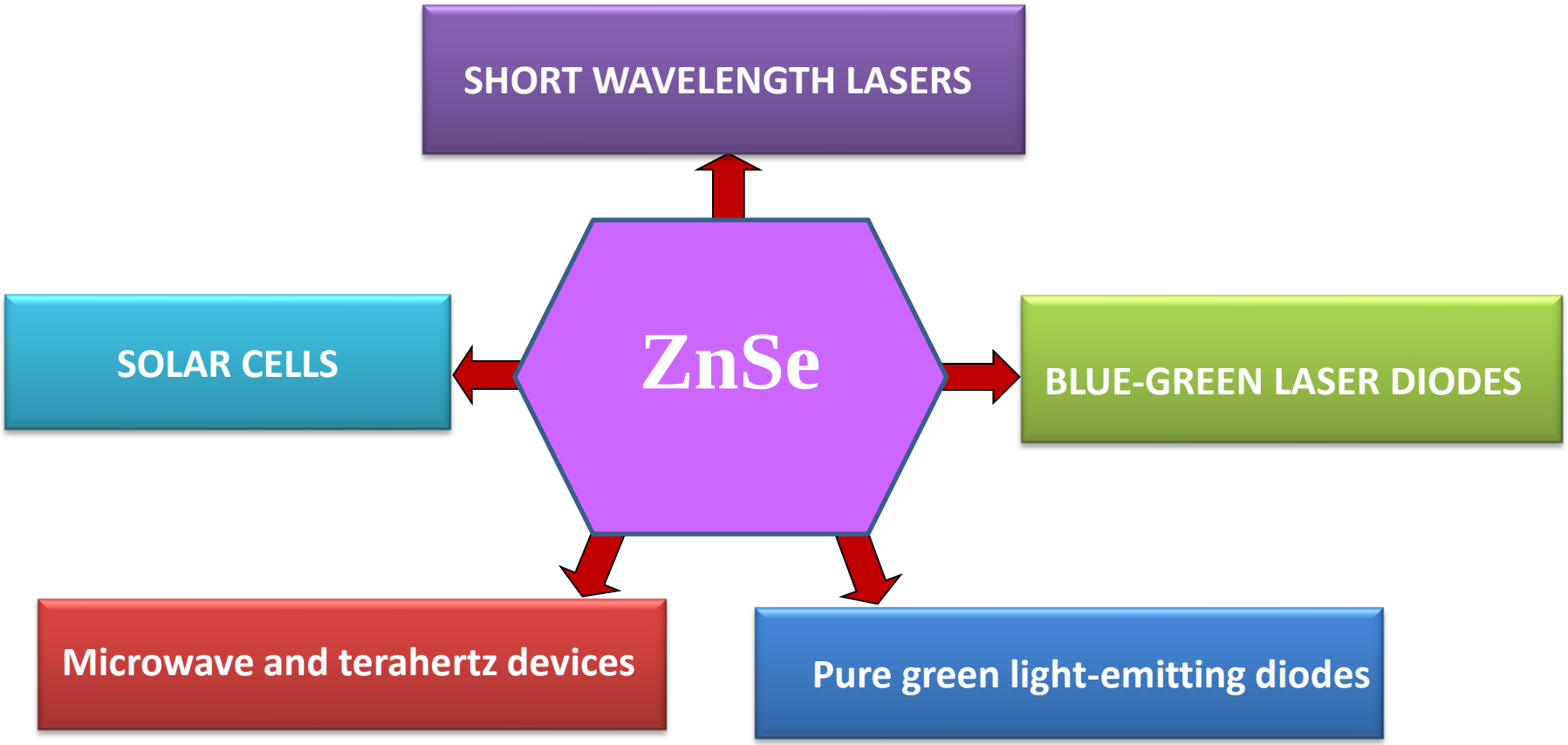
APPLİCATİONS



CALCULATION METHODS

This work is dedicated to study of the magnetism in ZnSe:Fe by varying the impurity concentrations for the values *x*=12.5 %, 6.25 %, 4.16 %, 2.08 %, using **local spin density gradient approximation** (LSDA) **and Hubbard U methods base on DFT [1]**.

A *k*-sampling Monkhorst-Pack grids 5×5×5 used and all atomic positions have been geometry optimized. The valence electron configurations which included 12 electrons for Zn [Ar] $+3d^{10}\ 4s^2$, 6 electrons for Se [Ar] $+4s^2\ 4p^4$ and Fe [Ar] $+3d^5\ 4s^1$ were taken into consideration. Hubbard U semiempirical corrections (U=4.5 eV on *d*-states of Zn and U=3.8 eV on *p*-states of Se) are used for correct band gap prognosis for bulk ZnSe. The simulations are carried out for different supercells generated with the initial lattice parameters *a*=*b*=3.98 Å and *c*=6.53 Å [2].

First-principle calculations carried out implementing Atomistic ToolKit code.

[1] Hohenberg P., Kohn W. Phys. Rev., 1964, v.136, p.B864-B871
[2] Wyckoff R W G (1963) Second Edition. Interscience Publishers, New York Note Cadmium Iodide Structure. Crystal Structures 1:239-444

Magnetic properties of $Zn_{1-x}Fe_xSe$

This work based on the DFT-LSDA+U, detailed theoretical study of magnetic properties for Fe^{2+} doped ZnSe structure is provided. In our previous work [1,2] obtained that the calculated energy band gap (2.7 eV) of ZnSe is closer to the known experimental results (2.70 eV).

Current studies show that a single Fe(Zn) substitution leads to magnetization and the magnetic moment for 96-atom systems is around 4 μ_B, which is consistent with the band structure results. In case of Fe(Zn), Zn atoms have a less weakening effect on the magnetic field (~ -0.05 μ_B), the magnetization created mainly by the impurity atom (~ 3.5 μ_B from Fe atom including 3.359 μ_B from *d*-electrons). The positive magnetic moments of all Se atoms (~ 0.6 μ_B) are small in magnitude.

Table 1. The DFT-LSDA+U results for $Zn_{1-x}Fe_xSe$.

Supercell	x	μ(Fe), μ_B per Fe	$(E_{AFM}-E_{FM})/2$, *meV* per Fe
$Zn_{15}Fe_1Se_{16}$	0.0625	4.004	-
$Zn_{14}Fe_2Se_{16}$	0.125	4.0	0.205
$Zn_{47}Fe_1Se_{48}$	0.0208(3)	4.0	-
$Zn_{46}Fe_2Se_{48}$	0.04166	3.9975	0.035

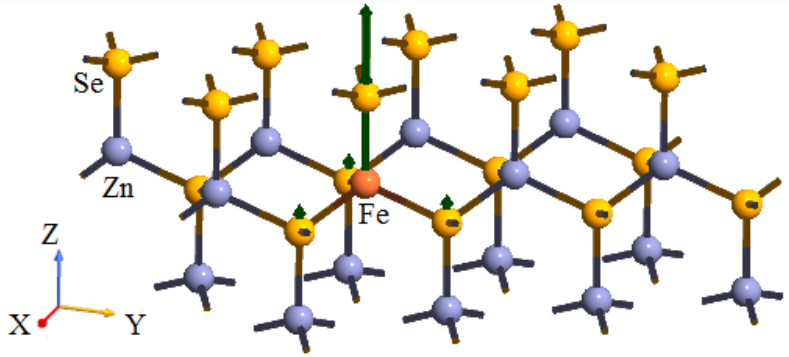


Fig.1. The spin-polarization for $Zn_{15}Fe_1Se_{16}$ supercell (Zn-gray, Se-yellow, Fe-brown).

[1] **Jafarova V N**, Orudzhev H S (2021) Structural and electronic properties of ZnO: A first-principles density-functional theory study within LDA(GGA) and LDA(GGA)+ U methods. Solid State Communications, 325:114166-114170

[2] **V.N. JAFAROVA**, M.A. MUSAEV: First-principles study of structural and electronic properties of ZnSe with wurtzite structure. *Technium: Romanian Journal of Applied Sciences and Technology,* 6, 42 (2023).

ZnSe:Fe with Zn vacancy-defect

For Fe(Zn) replacement and availability of one Zn vacancy positioned far from the impurity atom, the computed total moment of the 96-atom supercell is 5.594 μ_B, with main partial magnetic moments from Fe (3.607 μ_B) and 48 Se atoms (2.774 μ_B).

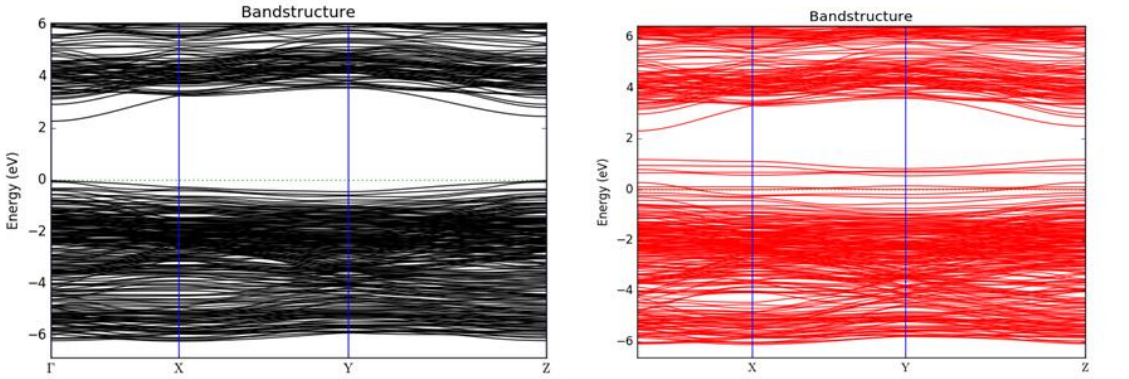


Fig.3. The calculated band structures of $Zn_{46}Fe_1Se_{48}$ (spin-up-black) and spin-down-red states).

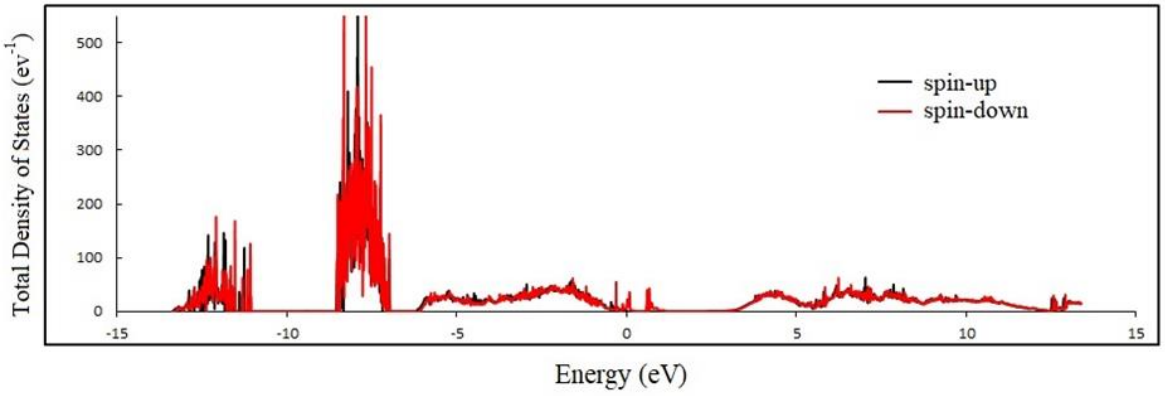


Fig.4. The DFT-LSDA+U calculated TDOS of $Zn_{46}Fe_1Se_{48}$ system with Zn vacancy.

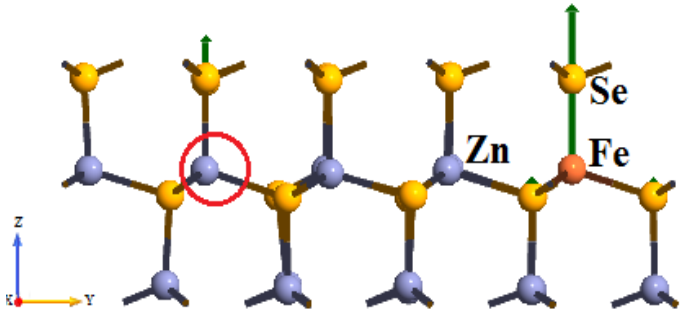


Fig.2. The spin polarization structure for $Zn_{14}Fe_1Se_{16}$.

The shift of moment of system due to one Zn vacancy side is (1.6 ÷ 1.9) μ_B depending on the chosen location of the defect.

CONCLUSİONS

- Using an accurate DFT-LSDA+U approach, have been explored the spin-polarized electronic and magnetic properties of defected Zn1-xFexSe. While the introduction of Fe2+ ions in the doped ZnSe systems change the spin-down bandstructure.

- Form the first-principles study obtained that the pure ZnSe is a non-magnetic direct band gap semiconductor. Investigations show that adding the iron and the presence of a single Zn vacancy-defect leads to the magnetization of ZnSe.

- The results of total energy calculations show that a ferromagnetic (FM) state is favorable when Zn is replaced with Fe. The FM alignment in Fe-doped ZnSe wurtzite compound behaves in high-spin and half-metallic states.

THANKS FOR YOUR ATTENTION !