High Curie temperature in Zn(Co,Ni)Se: First-principles study of correlation between chemical environment and ferromagnetism

International Conference on Sustainable Future and Environmental Science (EsiTech-2023)
Bucharest, Romania

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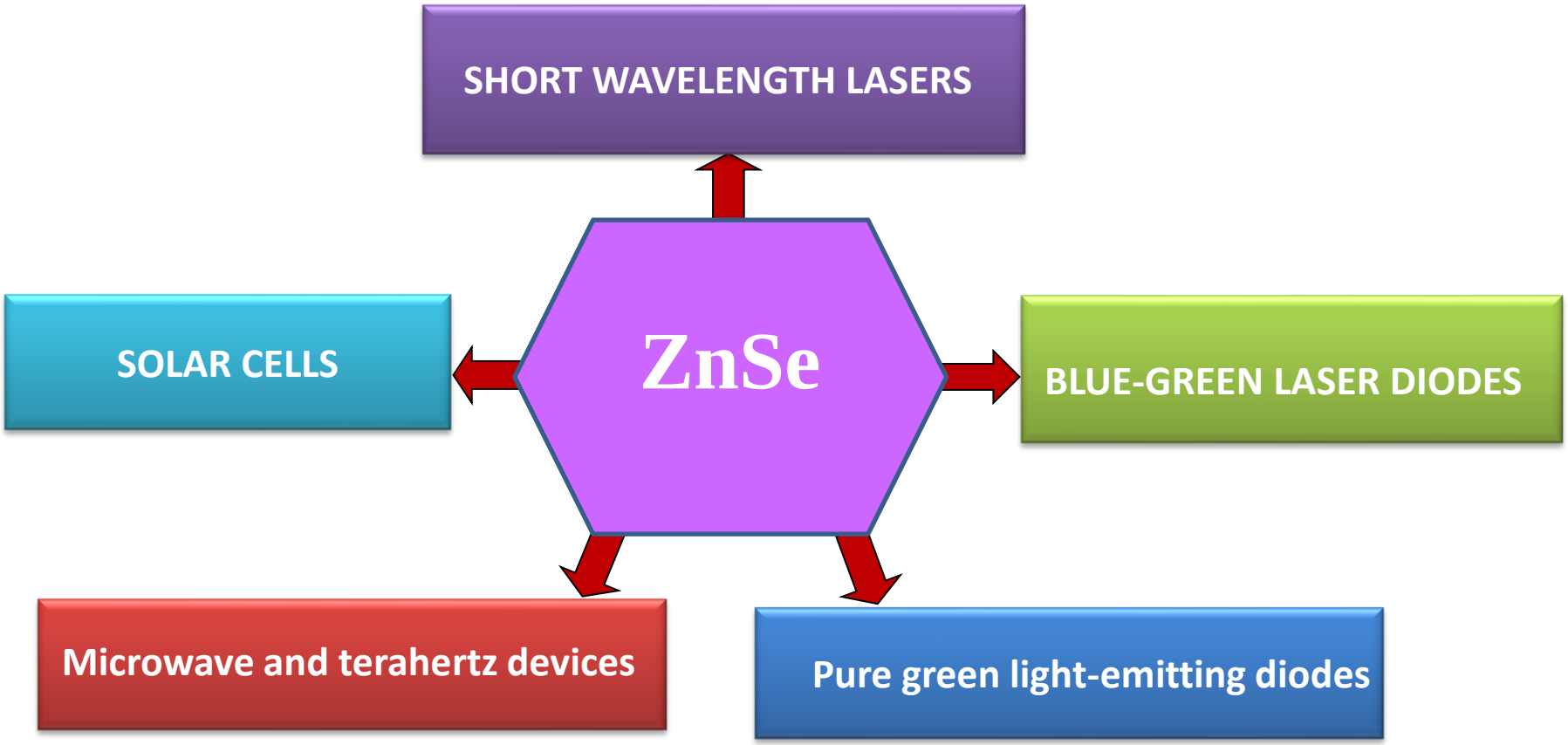
APPLİCATİONS



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] +$4s^2$ $4p^4$, 9 electrons Co [Ar] +$3d^7$ $4s^2$, and 10 electrons for Ni [Ar] +$3d^8$ $4s^2$ were taken into consideration. The kinetic cut-off energy of 100 Ry (50 Ha) was employed through-out the calculations which was tested to be fully converged with for to total energy. Magnetic properties were investigated after a full geometry optimization of all systems (for all lattice parameters and atomic positions) with force and stress tolerances of 0.01$eV/Å$ and 0.01 $eV/Å^3$, respectively.

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(Co)Se

Zinc selenide is a nonmagnetic material with a direct band gap of 2.70 eV and has great potential for a diversity of optical and electro-optical devices, such as short wavelength lasers, blue-green laser diodes, pure green light-emitting diodes, microwave and terahertz devices, solar cells and tunable mid-IR laser sources The first-principles calculated total magnetic moments of Co-doped ZnSe supercells are found to be equal to 3 μ_B

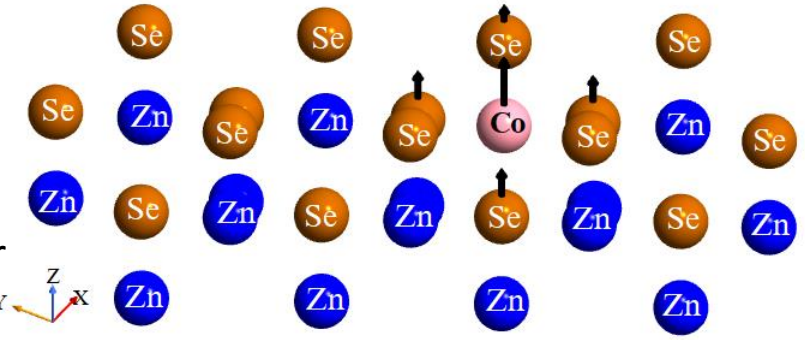


Fig.1. The spin-polarization of $Zn_{15}Co_1Se_{16}$.

Table 1. The Co-Co bond lengths and the total energy differences beetween AFM and FM alignments.

System	d_{Co-Co} [Å]	E_{AFM} [eV]	E_{FM} [eV]	ΔE [eV]
$Zn_{14}Co_2Se_{16}$	7.96	-30326.08060	-30326.05138	-0.02922
$Zn_{30}Co_2Se_{32}$	9.50	-61957.01379	-61957.01286	-0.00093

[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).

Magnetic properties of Zn(N)Se

In the case of Ni-doping ZnSe the obtained values of total and partial magnetic moments for supercell and per impurity atom are found to be equal 4 and 1.223 μ_B, respectively. The main contribution to the magnetization from *d*-states of Ni atom (~1.2 μ_B), the small negative contribution from 15 Zn atoms. The significant positive contribution from 4 Se atoms (0.85 μ_B) which chemically bonded nickel dopant atom.

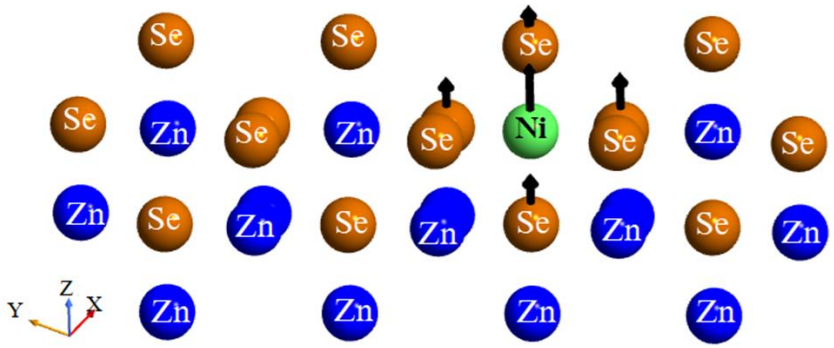


Fig.2. The spin-polarization of $Zn_{15}Ni_1Se_{16}$. Magnetic moments of atoms are shown by black arrows.

Table 2. The Ni-Ni bond lengths and the total energy differences beetween AFM and FM alignments

System	$d_{Ni\text{-}Ni}$ [Å]	E_{AFM} [eV]	E_{FM} [eV]	ΔE [eV]
$Zn_{14}Ni_2Se_{16}$	7.96	-30727.85236	-30727.97240	0.12004
$Zn_{30}Ni_2Se_{32}$	9.50	-62358.71828	-62358.74156	0.02328

Table 3. Calculated values of formation energies and the Curie temperatures for $Zn_{1-x}Co_xSe$ and $Zn_{1-x}Ni_xSe$ systems, per two Zn atoms replaced by Co^{2+} or Ni^{2+} ion.

System	*x*, %	$E_{form.}$[eV]	T_C [K]
$Zn_{14}Co_2Se_{16}$	12.5	40.92	-904
$Zn_{14}Ni_2Se_{16}$	12.5	28.35	3714

CONCLUSİONS

- Using an accurate DFT-LSDA+U approach, have been explored the spin-polarized electronic and magnetic properties of $Zn_{1-x}Co_xSe$ and $Zn_{1-x}Ni_xSe$ for x=12.5 %, 6.25 %. While the introduction of Ni^{2+} ion and the presence of Zn vacancy in ZnSe structure lead the half-metallic ferromagnetic coupling.
- For the Co-doped ZnSe systems are not observed half-metallic state. The obtained values of total magnetic moments have been found to be 3.0 and 4.0 μ_B for $Zn_{1-x}Co_xSe$ and $Zn_{1-x}Ni_xSe$, and the mainly contribution to the magnetization comes mostly from *d*-states of impurity atoms.
- Results of the energy differences between the antiferromagnetic and the ferromagnetic states for both systems nearly represent a stable ferromagnetic phase. The presence of Zn vacancy in ZnSe:Co systems affect the magnetization, which ~2.0 μ_B increases the total magnetic moment of the supercell (~5.0 μ_B).

THANKS FOR YOUR ATTENTION !