

Investigation on Electronic and Magnetic Properties of Transition Metals Doped Zinc Selenide

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Abstract : The full potential linear augmented plane wave (FPLAPW) based on density-functional theory (DFT) is employed to study the electronic, magnetic and optical properties of some transition metals doped ZnSe. Calculations are carried out by varying the doped atoms. Four 3D transition elements were used as a dopant: Cr, Mn, Co and Cu in order to induce spin polarization. Our results show that, Mn and Cu-doped ZnSe could be used in spintronic devices only if additional dopants are introduced, on the contrary, transition elements showing delocalized quality such as Cr, and Co doped ZnSe might be promising candidates for application in spintronic.

Keywords : spin-up, spin-down, magnetic properties, transition metal, composite materials

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