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Magnetic properties of Mn doped zinc selenide clusters: First principles calculations[1] SACHIN NANAVATI, Department of Electronic Science, University of Pune, Pune 411007 India, SUNDARARAJAN V., Centre for Development of Advanced Computing (C-DAC), Pune University campus, Pune 411007, India, SHAILAJA MAHAMUNI, Department of Physics, University of Pune, Pune 411007, India, SUBHASH GHAISAS, Department of Electronic Science, University of Pune, Pune 411007, India, VIJAY KUMAR, Dr. Vijay Kumar Foundation, 1969, Sector 4, Gurgaon 122001, India — We report the result of our study on magnetic properties of Mn doped ZnSe clusters within the pseudopotential based density functional theory (DFT). In the present work, we substituted one or two Mn atoms at different cationic sites of small ZnSe clusters and the corresponding stable geometrical configurations are obtained. In general, we find a large magnetic moment of 5 μ_B magnetic moment when one Mn atom is substituted. For the case of doping of two Mn atoms, calculations were performed for both parallel and anti-parallel spin-configurations. The variations in the density of state (DOS), the gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), the binding energy, and the magnetic moment have been analyzed as a function of the cluster size. This paper will discuss the preferred sites of the dopants, type of magnetization and their bonding characteristics for the above mentioned clusters.

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