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# Density functional calculations for manganese impurity in bulk silicon material

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ABSTRACT

Using the density functional theory within the spin generalised gradient approximation ($\sigma$GGA), we systematically investigate the structural, magnetic, and electronic properties of silicon crystal upon the influence of doping manganese atoms. We have also presented detailed results and comparison for the substitutional and interstitial Mn-doped structures. It is found that the tetrahedral interstitial site is the energetically most stable structure for the Mn-doped Si with a little energy preferency over the substitutional site. To account the effect of the electron correlation on the Mn 3d orbitals, we have carried out similar calculations by employing the Hubbard potential U within the standard GGA method (*viz.* $\sigma$GGA+U method). Finally we have compared the results obtained within these computational approaches, $\sigma$GGA and $\sigma$GGA+U, with the available theoretical and experimental findings.