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Density functional study of manganese doped bulk silicon[1] BHAGAWAN SAHU, Microelectronics Research Center, University of Texas at Austin, Austin, TX 78758, LEONARD KLEINMAN, Department of Physics, University of Texas at Austin, Austin, TX 78712, SANJAY BANERJEE, Microelectronics Research Center, University of Texas at Austin, Austin, TX 78758 — Using a 250 atom Si supercell with two manganese impurities at the substitutional and tetrahedral interstitial positions, we find, using the density functional projector-augmented wave method, that the ferromagnetic arrangement of manganese atoms at the tetrahedral interstitial position is energetically more stable compared to that at the substitutional position. We find a half-metallic density of states (integer spin magnetic moment over the supercell) for both the interstitial and substitutional manganese. However, the total energy difference (or magnetic energy difference) between interstitial manganese in the ferro and anti-ferro spin-alignments are not large enough to conclude whether ferromagnetic or antiferro-magnetic stability is preferred in the pure Si samples doped with manganese.

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