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Transition metal doped SiC: defect levels and magnetism[1] M.S. MIAO, WALTER R.L. LAMBRECHT, Case Western Reserve University — The properties of transition metal substitutions and interstitials in 3C and 4H SiC are studied by first principles supercell calculations. The defect levels change slightly for different polytypes or for different layers in 4H SiC. The calculated defect levels are generally in good agreements with DLTS results. Ti in 4H SiC has two acceptor levels close to the conduction band minimum, corresponding to cubic and hexagonal layers.V, Cr and Mn are amphoteric and have both donor and acceptor levels in the gap. We found Mn has deep trap levels which may be useful to achieve semi-insulating SiC, as is also well-known to be the case for V. The Cr and Mn acceptor levels are deep in the gap. They are unlikely to induce holes at the valence band maximum. Therefore the well-known hole-mediated ferromagnetic mechanism does not apply to Cr and Mn doped SiC. However, our calculations showed ferromagnetic coupling for Cr or Mn doped at neighboring sites. The ferromagnetic coupling is very strong but localized for Cr:SiC. However, it is relatively weak but long range for Mn:SiC. Such features are determined by the nature of the impurity bands. The highest occupied defect state of Cr:SiC is antibonding e which is localized whereas the state of Mn:SiC is $t2$ which is delocalized and strongly couples with the surrounding C dangling bonds.

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