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Studies of singly doping of Me and Fe in Si to deduce simple guidelines in selecting transition metal elements for Si-based spintronic materials MICHAEL SHAUGHNESSY, UC Davis/LLNL, C.Y. FONG, RYAN SNOW, UC Davis, LIN YANG, LLNL — Single dopings of Mn and Fe in Si are investigated using 8-, 64-, and 216-atom supercells and a first-principles method based on density functional theory. Atomic sizes play an essential role in determining the contraction or the expansion of neighboring atoms around the transition metal element at a substitutional site. At a tetrahedral interstitial site, there is only expansion. Magnetic moments/transition- metal-element at the two sites are calculated. Physical reasons for these properties are given. Some guidelines for selecting transition metal elements doped in Si for future Si-based effective spintronic materials are proposed.

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