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Electronic properties and magnetic moments of Mn_xSi_{1-x} for x < 5%. MICHAEL SHAUGHNESSY, RYAN SNOW, CHING YAO FONG, University of California Davis Physics Department — Recently, there have been experimental reports about Mn_xSi_{1-x} alloys. All show great promise for room temperature spintronic applications. We report on theoretical studies of the electronic properties of Mn_xSi_{1-x} for x < 5%, using first principles density functional methods. For the Mn-doped Si, we consider three configurations of the Mn impurities: nearest neighbor (nn), second nearest neighbor (snn), and a three-atom chain configuration. For the nn and snn configurations, the ferromagnetic and antiferromagnetic phases have been compared. The magnetic moment/unit-cell for the nn and ferromagnetic configurations is smaller than for the ferromagnetic snn and chain configurations. The reason will be given. Supported in part by NSF grant: ESC-0725902.

Michael Shaughnessy
University of California Davis Physics Department

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