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Mn-doped monolayer MoS_2: An atomically thin dilute magnetic semiconductor DORON NAVEH, Department of Electrical Engineering and The Institute for Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat-Gan 52900, Israel, ASHWIN RAMASUBRAMANIAM, Department of Mechanical and Industrial Engineering, University of Massachusetts Amherst, Amherst, Massachusetts 01003, USA — We investigate the electronic and magnetic properties of Mn-doped monolayer MoS_2 using a combination of first-principles density functional theory (DFT) calculations and Monte Carlo simulations. Mn dopants that are substitutionally inserted at Mo sites are shown to couple ferromagnetically via a double-exchange mechanism. This interaction is relatively short ranged, making percolation a key factor in controlling long-range magnetic order. The DFT results are parameterized using an empirical model to facilitate Monte Carlo studies of concentration- and temperature-dependent ordering in these systems, through which we obtain Curie temperatures in excess of room temperature for Mn doping in the range of 10–15%. Our studies demonstrate the potential for engineering a new class of atomically thin dilute magnetic semiconductors based on Mn-doped MoS_2 monolayers.

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