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Interstitial Mn in Si: half-metallic heterostructures studied by density-functional theory PETER KRATZER, University Duisburg-Essen, D-47048 Duisburg, Germany, HUA WU, University Cologne, D-50937 Cologne, Germany, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, D-14195 Berlin, Germany — Adding magnetic functionality to the most common semiconductor, Si, is in its infancy. So far, research on Mn-doped Si has concentrated on substitutional Mn (Mn_{sub}) as done for Mn-doped GaAs and Ge, although Mn_{sub} impurities in Si are energetically less stable than interstitial Mn (Mn_{int}). In this work, we investigate the role of Mn_{int} impurities for ferromagnetism in Si, and propose a novel type of heterostructures with Mn_{int} δ-doping. Using density-functional theory within the generalized gradient approximation, we show that Si-based heterostructures with 1/4 layer δ-doping of Mn_{int} are half-metallic. For Mn_{int} concentrations of 1/2 or 1 layer, the δ-doped heterostructures still display a high spin-polarization of conduction electrons, about 85% and 60%, respectively. The proposed heterostructures are more stable than previously assumed δ-layers of Mn_{sub}. Contrary to wide-spread belief, the present study demonstrates that interstitial Mn can be utilized to tune the magnetic properties of Si, and thus provides a new clue for Si-based spintronics materials.

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