

Abstract Submitted
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Dopant-assisted Concentration Enhancement of Substitutional Mn in Si and Ge¹ WENGUANG ZHU, Harvard University & The University of Texas at Austin & The University of Tennessee, ZHENYU ZHANG, ORNL & The University of Tennessee, EFTHIMIOS KAXIRAS, Harvard University — Incorporation of Mn atoms as magnetic impurities in bulk Si and Ge is of great importance for integrating magnetism with existing device technology. Here, we study the influence of p- and n-type electronic dopants on Mn incorporation in bulk Si and Ge, using first-principles calculations within density functional theory. We find that in bulk Si, the site preference of a single Mn atom is changed from interstitial to substitutional in the presence of a neighboring n-type dopant (P, As, Sb). In bulk Ge, a Mn atom is more easily incorporated into the lattice when an n-type dopant is present in its immediate neighborhood, forming a stable Mn/dopant dimer with both impurities at substitutional sites. A detailed analysis of magnetic exchange interactions between such dimers reveals that magnetic properties are not degraded when Mn atoms coexist with n-type dopants.

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Wenguang Zhu
Harvard University & The University of Texas at Austin & The University of Tennessee

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