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Ferromagnetic ordering of Mn-As co-doped Ge as diluted magnetic semiconductors studied within a Heisenberg model¹ HUA CHEN, U of Tennessee-Knoxville, WENGUANG ZHU, ZHENYU ZHANG, U of Tennessee-Knoxville;Oak Ridge National Laboratory — To achieve room temperature ferromagnetism in group-IV-based dilute magnetic semiconductors, it is required to increase the concentration of the magnetic dopants in the host semiconductors. A recent theoretical study has suggested that the concentration of substitutional Mn in Ge can be greatly enhanced upon co-doping with As, an n-type electronic dopant [1]. Using Monte Carlo simulations based on a classical Heisenberg model with the magnetic coupling parameters calculated from first principles, we study the magnetic property of Mn and As co-doped Ge at low doping concentrations. The estimated Curie temperature increases almost linearly with increasing Mn doping concentration and reaches 264K at 5% Mn. In contrast, at the same doping level pure Mn doped Ge does not show any finite temperature ferromagnetic ordering. [1] W. G. Zhu, Z. Y. Zhang, and E. Kaxiras, Phys. Rev. Lett. 100, 027205 (2008).

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