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Exotic magnetic properties of diluted magnetic binary chalcogenides MAIA G. VERGNIORY, Max Planck Institute of Microstructure Physics, XABIER ZUBIZARRETA, Max Planck Institute of Microstructure Physics, 06120 Halle, Germany, MIKHAIL M. OTROKOV, Tomsk State University, 634050 Tomsk, Russia, IGOR V. MAZNICHENKO, JÜRGEN HENK, Institut für Physik, Martin-Luther-Universität Halle-Witternberg, 06009 Halle, Germany, EVGUENI V. CHULKOV, Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain, ARTHUR ERNST, Max Planck Institute of Microstructure Physics, 06120 Halle, Germany — Using first-principles Green function approach we studied electronic and magnetic properties of diluted magnetic binary chalcogenides A_2B_3 , doped with transition metals substituing the A element. The electronic structure of the impurities in the chalcogenides is mainly featured by the crystal field splitting. We found that two main mechanisms are responsible for long-range magnetic order in these materials: hole mediated magnetism within the layer of A atoms and indirect interaction between magnetic moments via a B atom. We also estimated Curie temperature of these systems, which was found in good agreement with the available experimental data. Our results shed light on the understanding of magnetic interaction and control in toplogical insulators.

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