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ABSTRACT:

Doping-Induced Magnetism and Half-Metallicity in Nanoribbons of Quartic Dispersion Materials

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Two-dimensional (2D) materials with quartic dispersion are known to develop magnetization upon doping. Here, we conduct a systematic investigation of magnetization in hole-doped quartic dispersion materials (GaS, InSe, TiO2), focusing on the effects of structural confinement from two-dimensional (2D) monolayers to quasi-one-dimensional nanoribbons (NRs). Upon hole doping, these NRs develop itinerant magnetization across a broad range of carrier densities and display half-metallic behavior. The spin-polarization energies of these NRs are remarkably enhanced relative to their 2D counterparts, with maximum increase being in the case of TiO2 from 31 to 103 meV/carrier. The spin-polarization energy strongly depends on the degree of localization of the magnetic moments along the width of NRs, which is determined by edge passivation and ribbon width. Strong deformation of the topmost valence bands at higher dopings indicates deviation from the Stoner mechanism.