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Structural and electronic phase transitions in ferromagnetic monolayer VS_2 induced by charge doping NANNAN LUO, Department of Physics, Tsinghua University, CHEN SI, School of Materials Science and Engineering, Beihang University, WHENHUI DUAN, Department of Physics, Tsinghua University — Among the known transition metal dichalcogenides (TMDs), monolayer VS_2 has attracted particular interest because of its intrinsic ferromagnetism and promising applications as a high-performance functional nonomaterial. Here, using first-principles calculations, we study the electronic and structural phase transitions in the monolayer VS_2 induced by charge doping. At the ground state, monolayer VS_2 is stabilized in the 2H phase, being a bipolar magnetic semiconductor (BMS) whose valence and conduction states near the Fermi level carry opposite spin polarization. With the increase of hole doping concentration, VS_2 will first experience an electronic phase transition from a BMS to a half metal, followed by a 2H-to-1T structural phase transition which concomitantly results in another electronic phase transition from the half metal to a normal metal. However, the electron doping can only induce the BMS-to-half metal electronic transition but will not trigger the structural phase transition. The completely different effects of electron and hole doping on the structural phase transition can be well explained by the energy band diagrams of VS_2. These results clearly establish the potential for VS_2 utilization in innovative phase-change electronic and spintronic devices.

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