Electronic structure and magnetothermal property of the Janus VSeTe monolayer manipulated by carrier doping

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ABSTRACT: Two-dimensional (2D) ferromagnetic materials with high magnetic crystalline anisotropy energy and high Curie temperature are in highly demand for magnetic storage devices. In this work, we employ first-principles calculations and Monte Carlo simulations to systematically investigate the crystalline structure, electronic, and magnetic properties of the Janus VSeTe monolayer under different carrier concentrations. It is found that, under appropriate carrier doping, the Janus VSeTe monolayer undergoes a transition from a semiconductor to a half-metal with 100% spin polarization. The obtained magneto crystalline anisotropy energy is 1157.72 μeV, and the easy magnetic axis undergoes a transition from in-plane to out-of-plane under hole doping. In addition, the Janus VSeTe monolayer exhibits a valley splitting of 86 meV and a Curie temperature of 454 K. Under hole doping, the valley

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splitting increases to 110 meV and the Curie temperature rises to 510 K. The coercivity calculated from the hysteresis loop is 0.13 T, and its hysteresis loss is low, showing its rapid response to external magnetic fields. Our work demonstrates the broad application potential of the Janus VSeTe monolayer in spintronic devices and provides theoretical support for future experiments.

Keywords: VSeTe monolayer; Ferromagnetism; Spintronics; Magnetothermal properties; First-principles calculations; Monte Carlo simulations

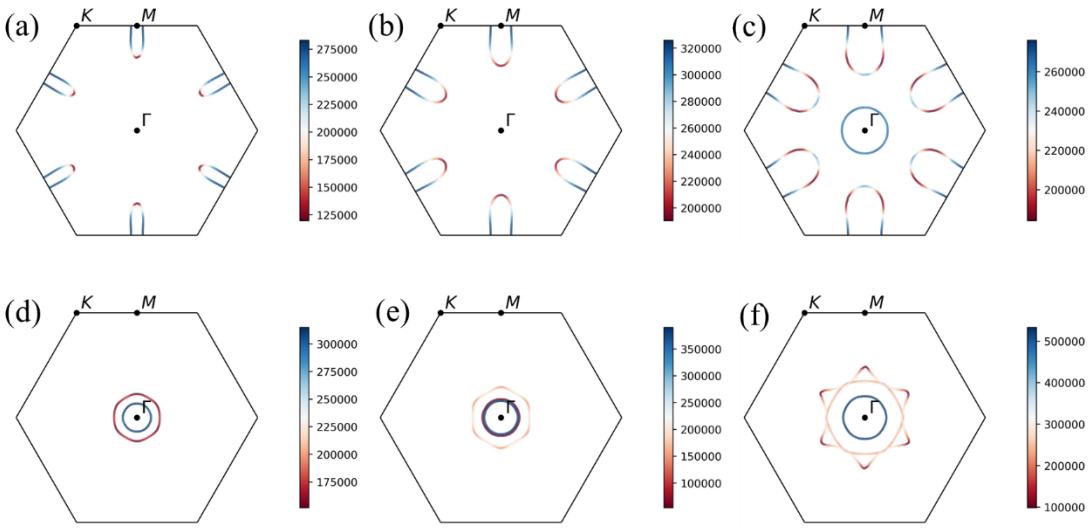

Fig. S1 (Color online) Fermi velocity projected Fermi surface under different carrier concentrations. (a) n = 0.02. (b) n = 0.04. (c) n = 0.1. (d) n = -0.02. (e) n = -0.04. (f) n = -0.1.

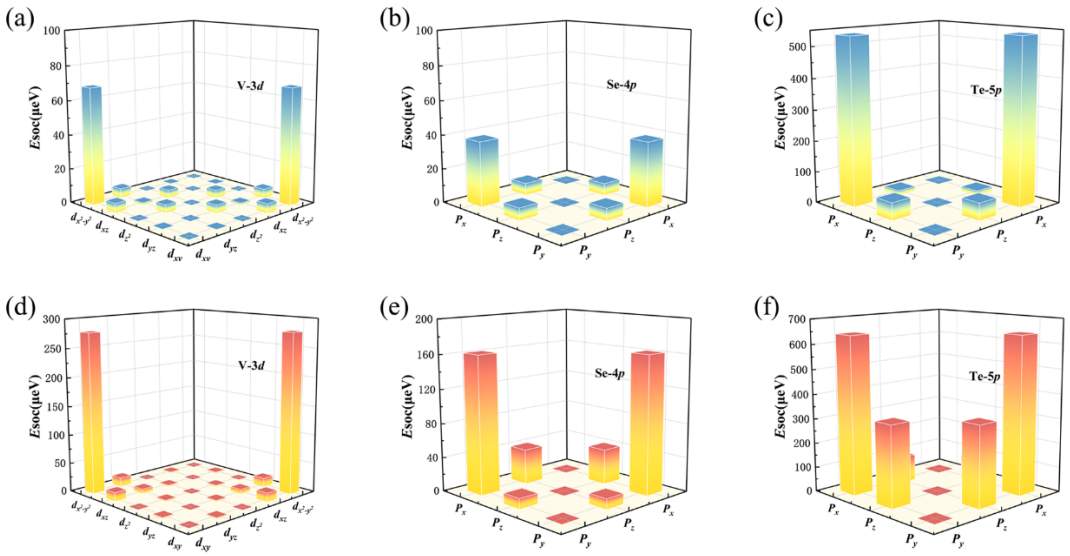

Fig. S2 (Color online) (a)–(c) The contribution of SOC deriving from the 5*p* of Te, 4*p* of Se and 5*p* of Te when the carrier concentrations are up to 7.293×10^{13} cm^{-2}(0.08 electrons per atom). (d)–(f) The contribution of SOC deriving from the 5*p* of Te, 4*p* of Se and 5*p* of Te when the carrier concentrations are up to 7.293×10^{13} cm^{-2}(0.08 holes per atom).

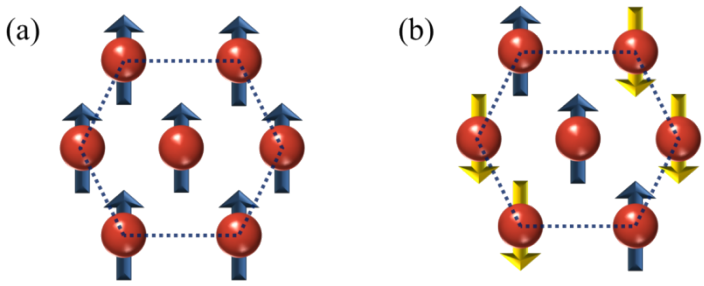

Fig. S3 (Color online) (a) FM configuration of the Janus VSeTe monolayer. (b) AFM configuration of the Janus VSeTe monolayer.

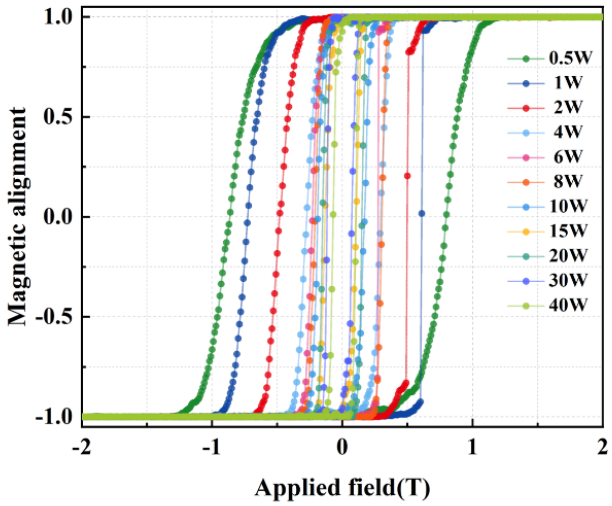

Fig. S4 (Color online) The lagging loop changes with the number of relaxation steps.

Table SI Energy differences between FM and AFM states, the variation in bond angles $\theta(^{\circ})$, and bond lengths d (Å) of the Janus VSeTe monolayer at different doping concentrations.

Carrier per atom	Δ_{AFM-FM} (meV)	θ_{V-Se-V} ($^{\circ}$)	θ_{V-Te-V} ($^{\circ}$)	d_{V-Se} (Å)	d_{V-Te} (Å)	d_{V-V} (Å)
-0.04	0.262	87.075	77.957	2.495	2.732	3.437
-0.02	0.391	87.013	78.325	2.496	2.721	3.437
0.00	0.183	87.010	78.701	2.496	2.710	3.437
0.02	0.154	86.973	78.857	2.497	2.706	3.437
0.04	0.118	86.948	79.000	2.498	2.702	3.437