Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Engineering the electronic and magnetic properties of d^0 2D dichalcogenide materials through vacancy doping and lattice straining

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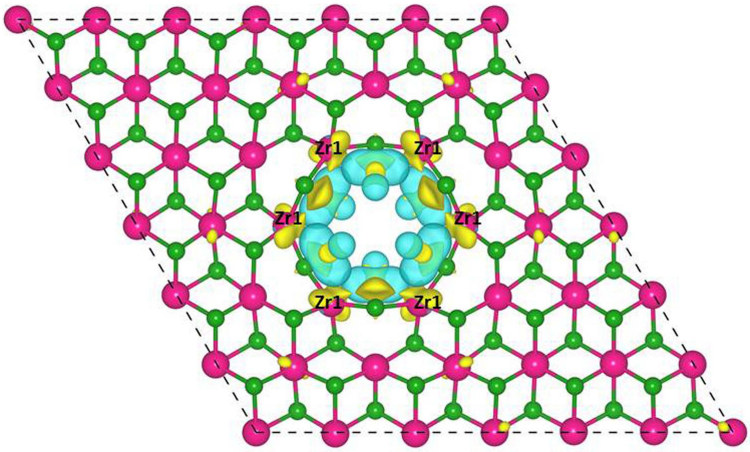

Fig. S1 Charge density difference of V-ZrS6 doped ZrS_2 monolayer. The yellow and blue isosurfaces show the electron accumulation and depletion, respectively. The isosurface value is taken as 0.004 eV/Å^3. The atoms color coding is the same as in Fig. 1.

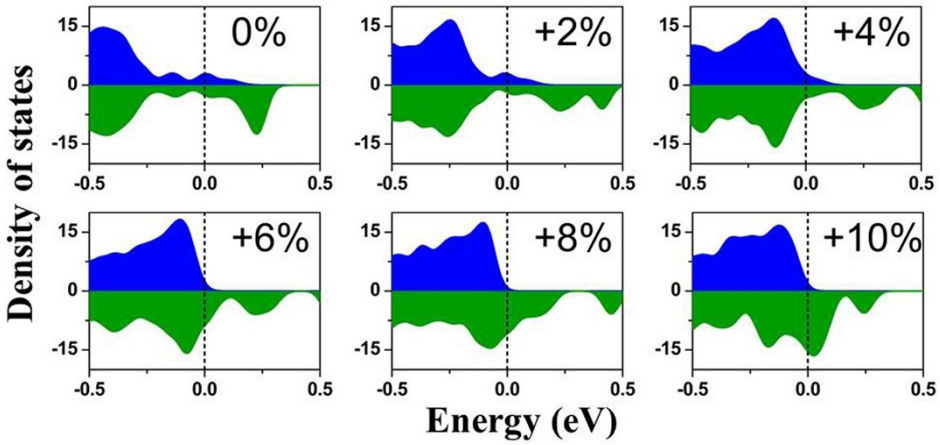

Fig. S2 Partial density of states for S-atoms *p* orbitals in V-Zr doped ZrS_2 monolayer at the energy window of -0.5 eV to 0.5 eV. The spin up and spin down parts are shaded by blue and green colors, respectively. The Fermi levels are all set to zero, which are indicated by black dashed line.

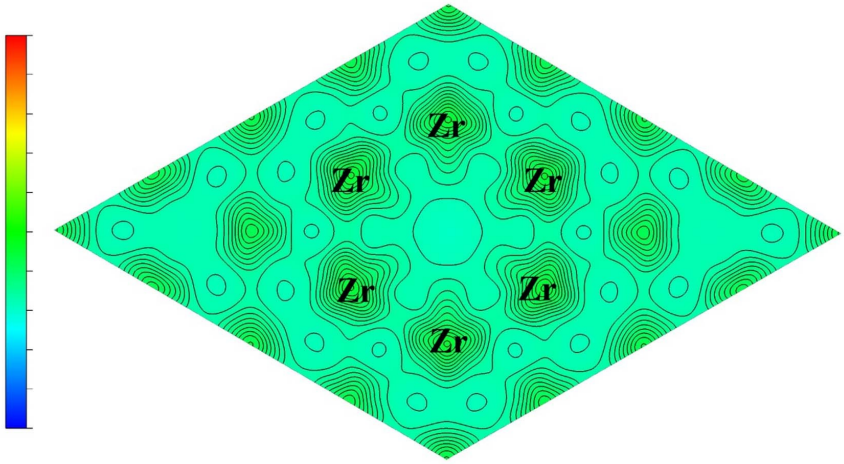

Fig. S3 Partial charge density projected on the Zr atom plane at the energy range from -1 eV to 0 eV relative to the Fermi level for the V-Zr doped ZrS_2 monolayer at the -8% strain.