Supporting Information

Epitaxial growth and electronic properties of antiferromagnetic semiconducting VI_2 Monolayer

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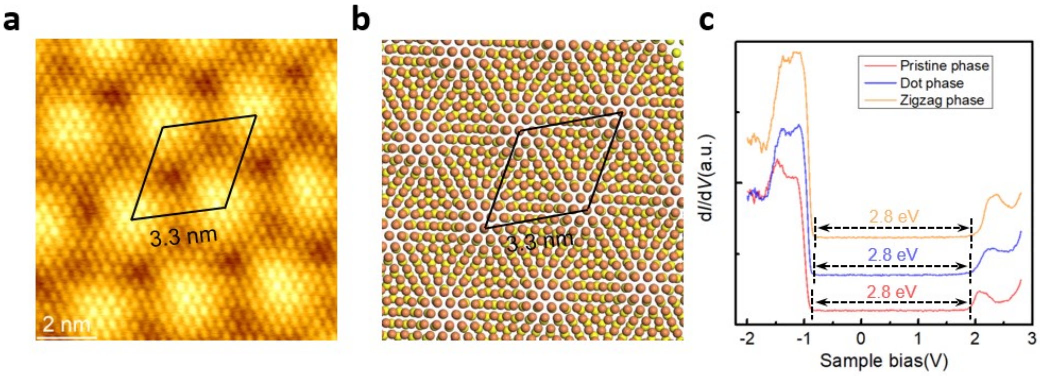


Fig. S1 Moire superstructures formed by single-layer VI_2 on iodine buffer layer. (a, b) The feasible schematic illustration of the dot phase. Yellow balls are iodine atoms of buffer layer on Au(111), and its period is 4.59 Å. Orange balls are iodine atoms in the bottom layer of VI_2, the other atoms are not displayed for simplicity. The Moiré pattern with periodicity of ~ 3.3 nm, it is consistent with the experimental results. (c) The dI/dV spectra obtained on different Moire superstructures have a band gap of 2.8 eV and no obvious difference was observed.

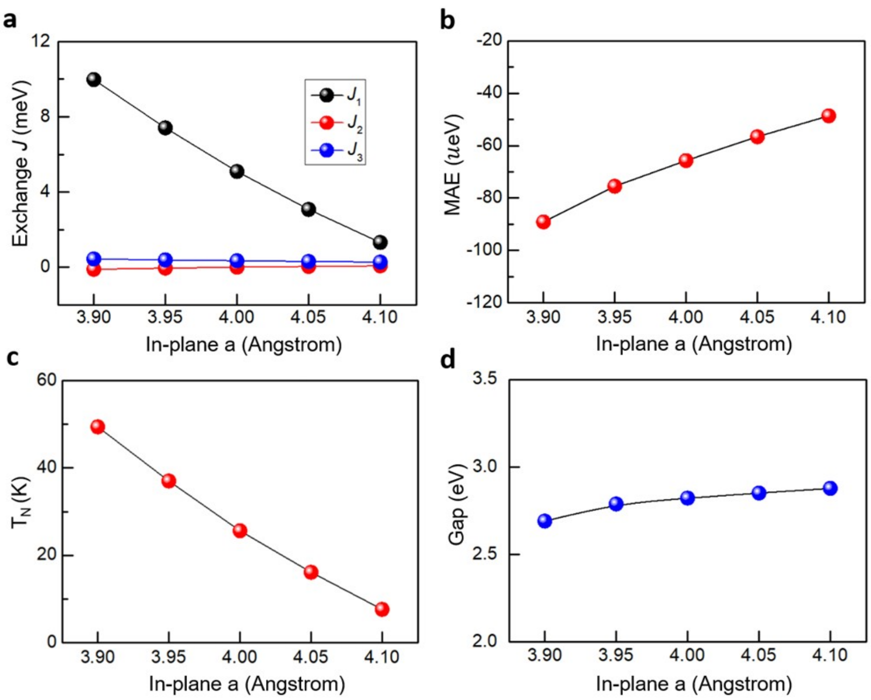
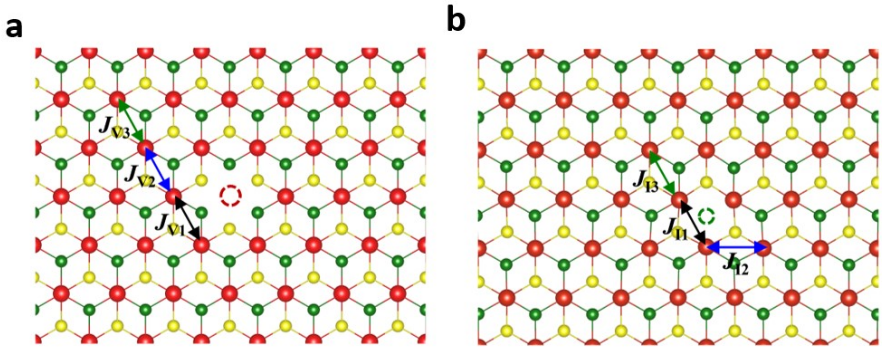


Fig. S2 Magnetic properties of VI_2 ML regulated by in-plane lattice constants. (a to d) DFT calculated exchange *J Néel* temperature T_N, magnetic anisotropy energy (MAE) and gap as a function of in-plane a.



$J_{V1} = -2.96$ meV

$J_{V2} = 0.82$ meV

$J_{V3} = 5.08$ meV

$J_{I1} = -24.15$ meV

$J_{I2} = 5.84$ meV

$J_{I3} = 4.49$ meV

Fig. S3 The Heisenberg exchange interactions between V^{2+} ions near vanadium and iodine vacancy defects. (a) Top view of one V vacancy defect in the 5 × 5 supercell VI_2 ML. The V vacancy defect is shown by the red empty circle. The back, blue and green double arrowed lines represent the considered Heisenberg exchange interactions J_{V1}, J_{V2} and J_{V3} that are near the V vacancy defect. (b) Top view of one I vacancy defect in the 5 × 5 supercell VI_2 ML. The I vacancy defect is shown by the green empty circle. In (a) and (b), red, green and yellow balls represents V, upper and bottom I atoms, repsectively. The back, blue and green double arrowed lines represent the considered Heisenberg exchange interactions J_{I1}, J_{I2} and J_{I3} that are near the I vacancy defect.