Supplementary Information (SI) for Nanoscale Advances.
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A systematic study of TMO_n (TM = V, Cr, Mn, and Fe; n = 3 and 6) cluster embedded in PtS_2 monolayer

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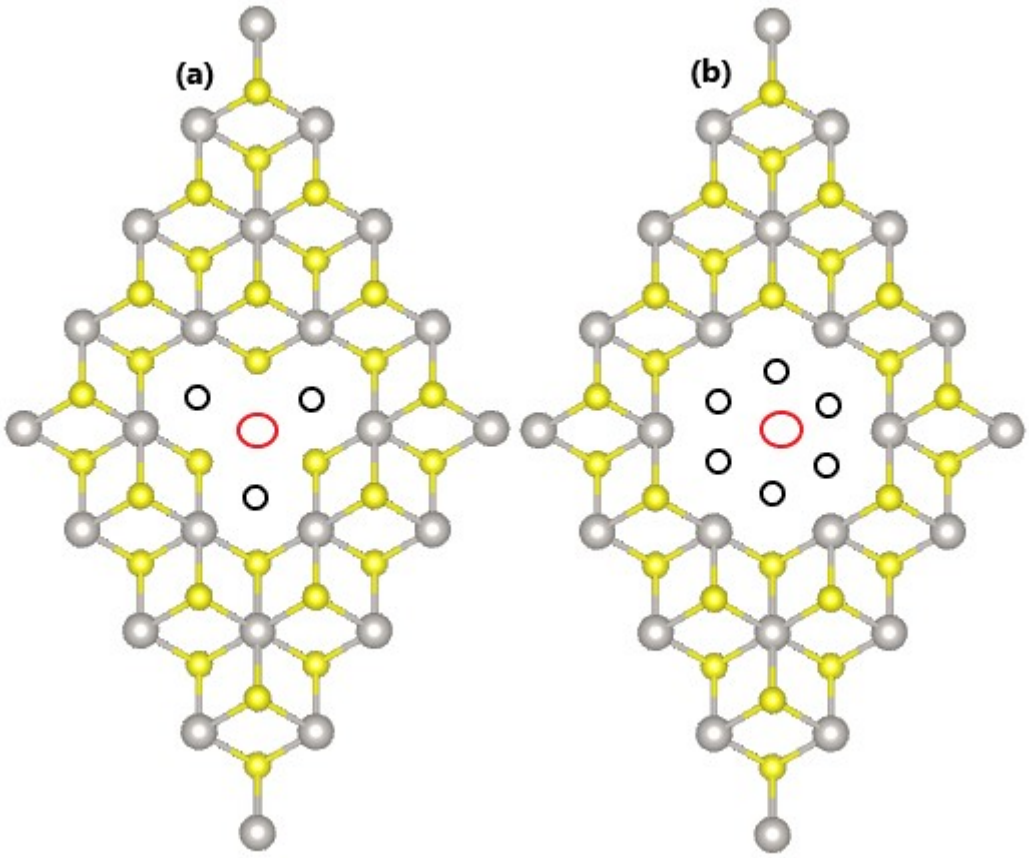

Figure S1: Atomic structure of PtS_2 monolayer with (a) PtS_3- and (b) PtS_6-type multivacancies (Red circle: Pt vacancy; Black circle: S vacancy).

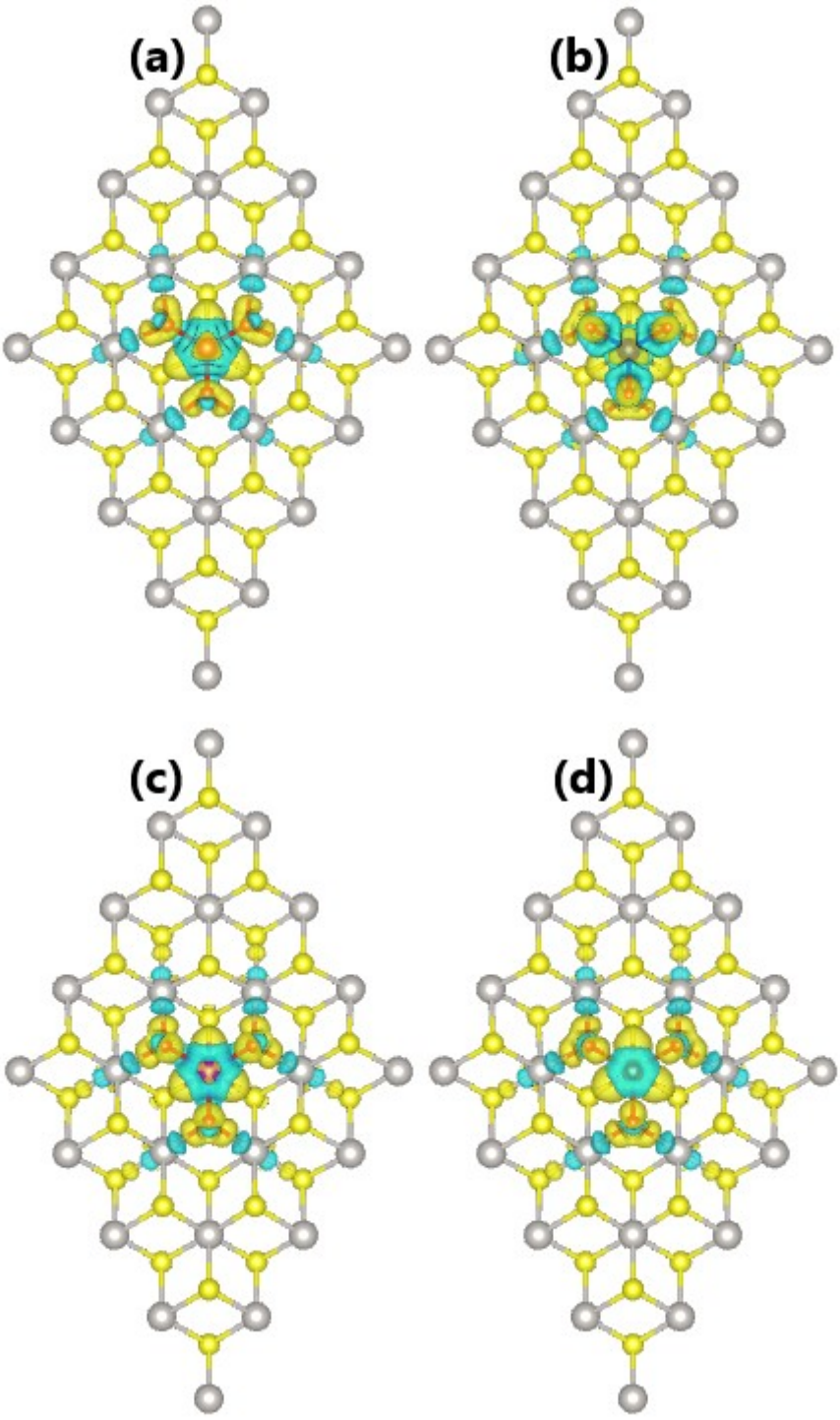

Figure S2: Charge density difference (Iso-surface value: 0.005 *e*/Å^3; Yellow surface: charge accumulation; Aqua surface: charge depletion) in PtS_2 monolayer doped with (a) VO_3, (b) CrO_3, (c) MnO_3, and (d) FeO_3 cluster.

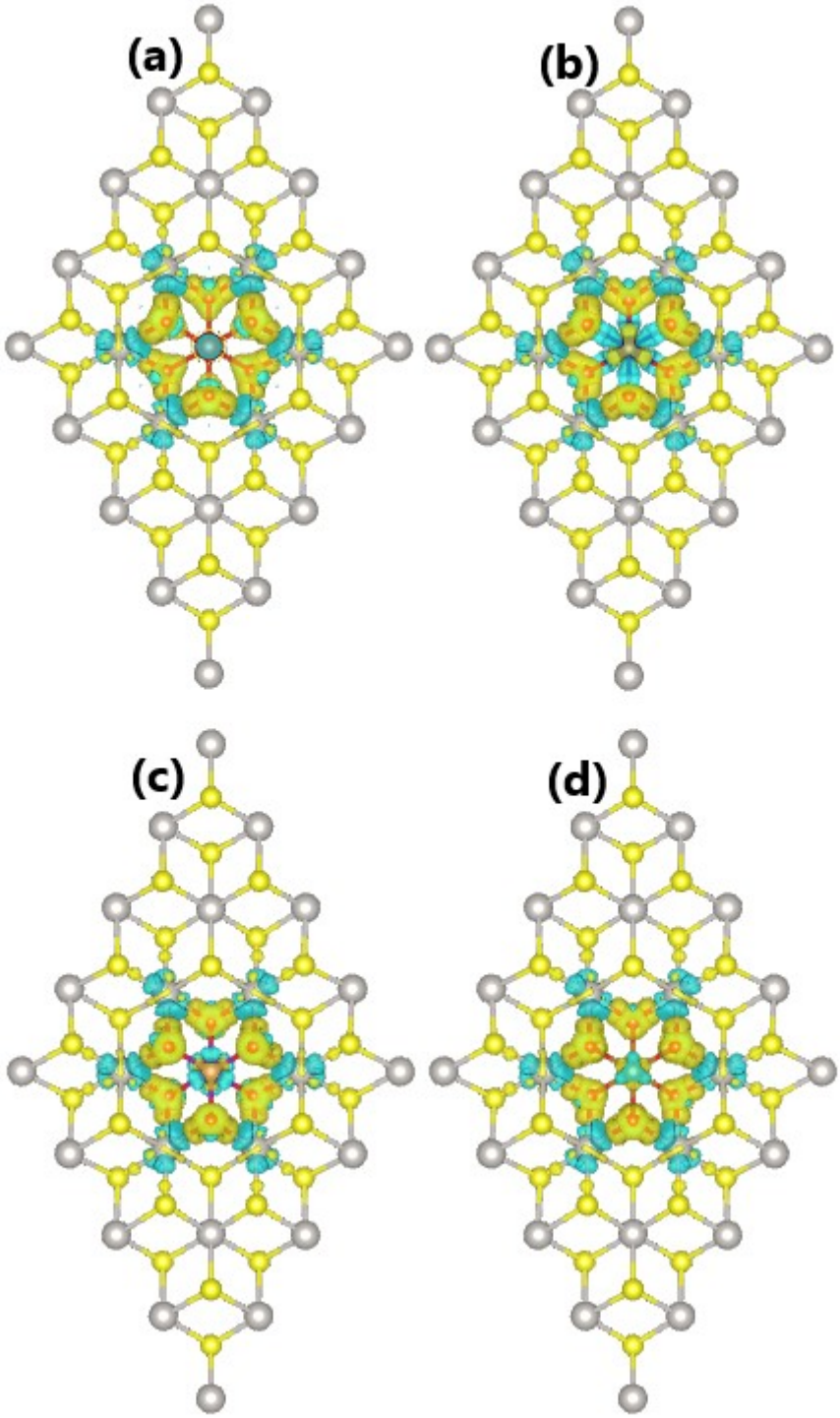

Figure S3: Charge density difference (Iso-surface value: 0.005 *e*/Å^3; Yellow surface: charge accumulation; Aqua surface: charge depletion) in PtS_2 monolayer doped with (a) VO_6, (b) CrO_6, (c) MnO_6, and (d) FeO_6 cluster.