

Vacancy-and doping-mediated electronic and magnetic properties of PtSSe monolayer towards optoelectronic and spintronic applications

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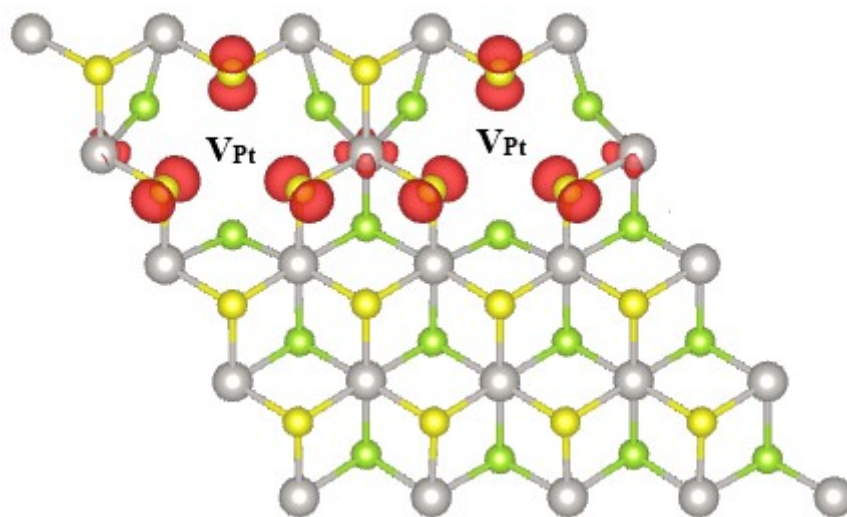


Figure S1: Spin density (Iso-surface value: $0.01 e/\text{\AA}^3$) in PtSSe monolayer with 12.5% of Pt vacancy.

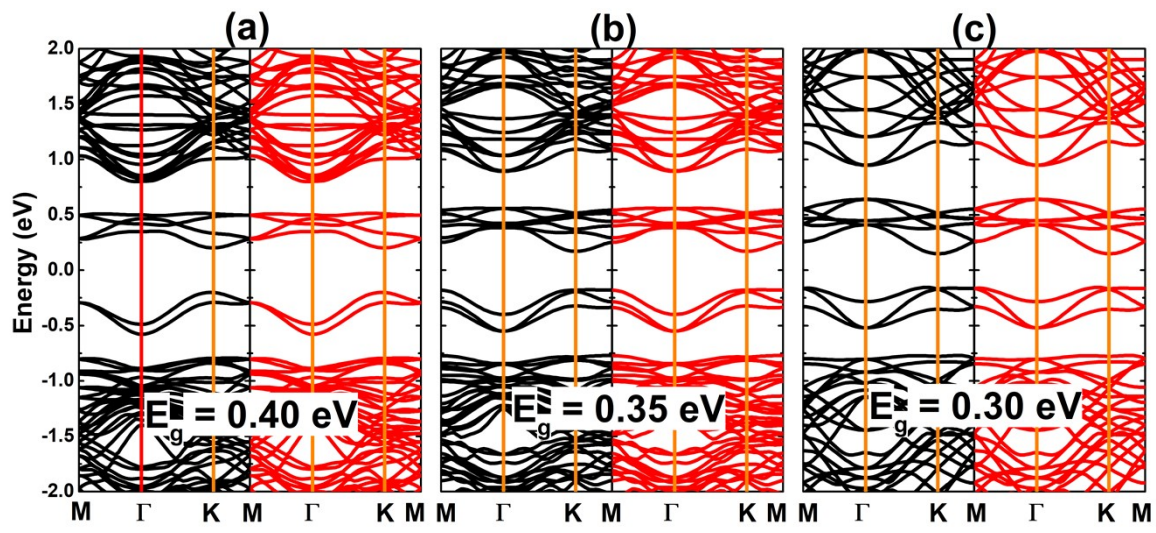


Figure S2: Spin-polarized band structure of PtSSe monolayer with (a) 12.5%, (b) 18.75%, and (c) 25% of S vacancy.

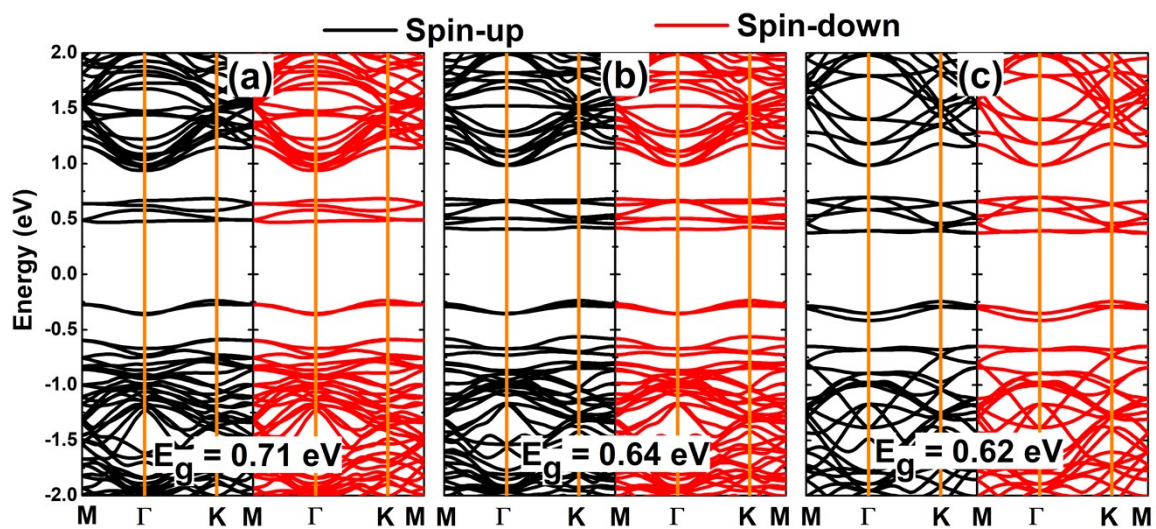


Figure S3: Spin-polarized band structure of PtSSe monolayer with (a) 12.5%, (b) 18.75%, and (c) 25% of Se vacancy.

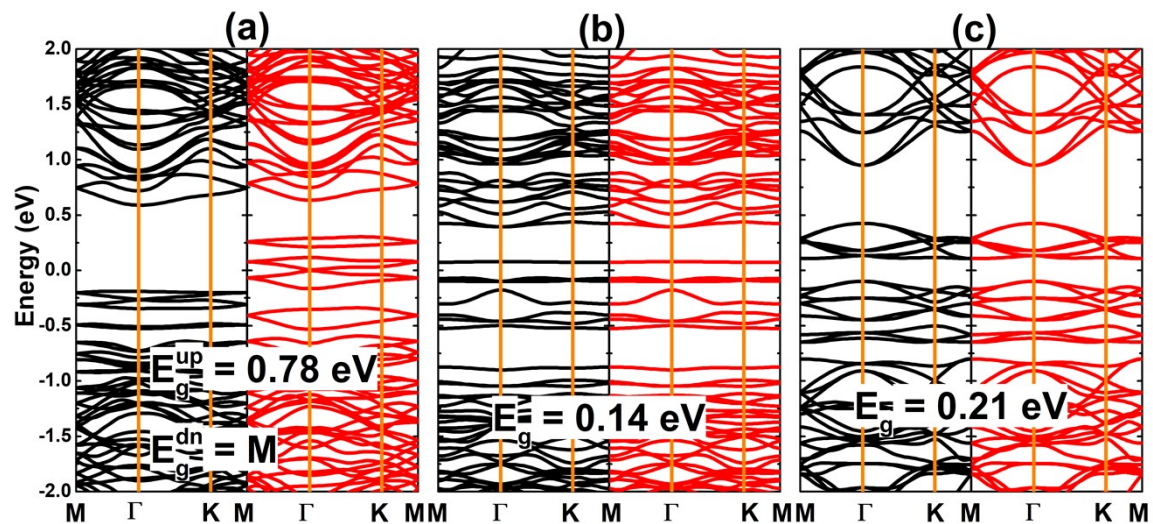


Figure S4: Spin-polarized band structure of PtSSe monolayer with (a) 12.5%, (b) 18.75%, and (c) 25% of Pt vacancy.

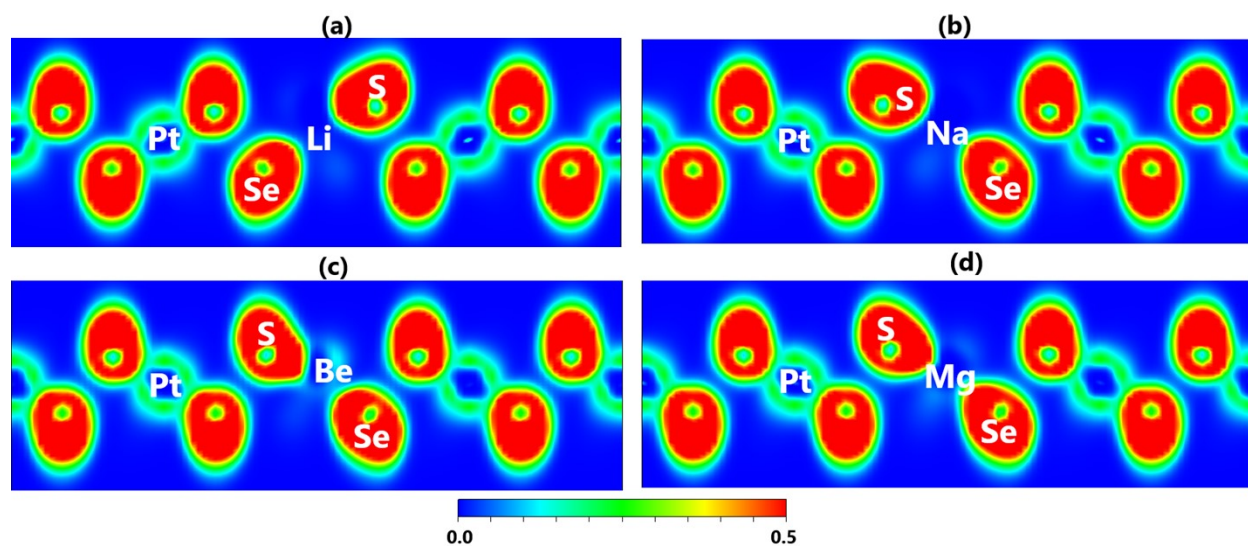


Figure S5: Electron localization functional in (a) LiPt , (b) NaPt , (c) BePt , and (d) MgPt system.

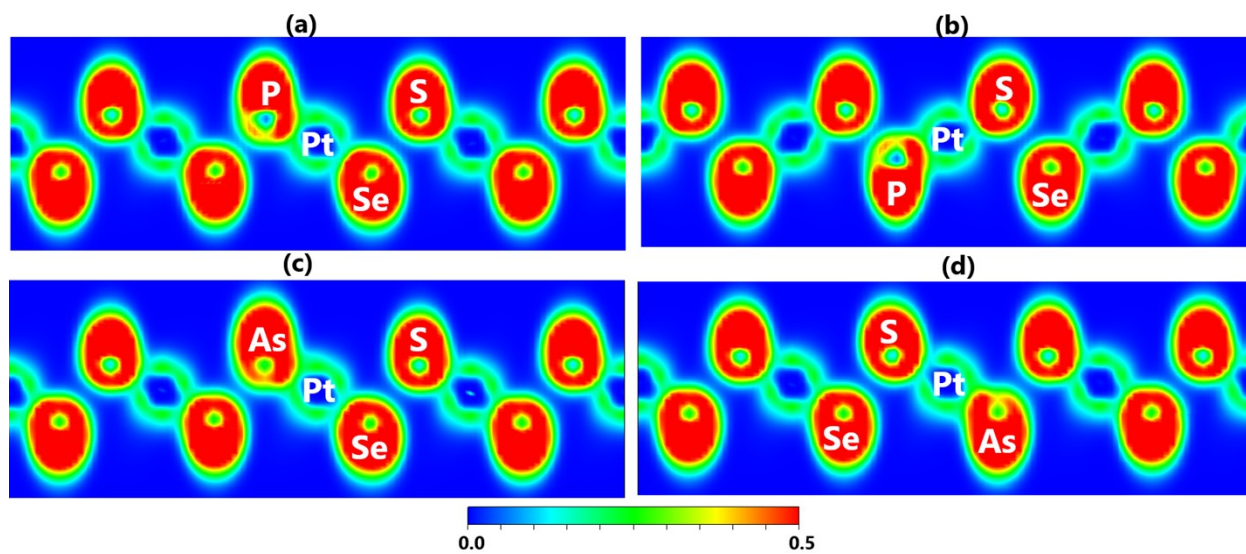


Figure S6: Electron localization functional in (a) P_S , (b) P_{Se} , (c) As_S , and (d) As_{Se} system.

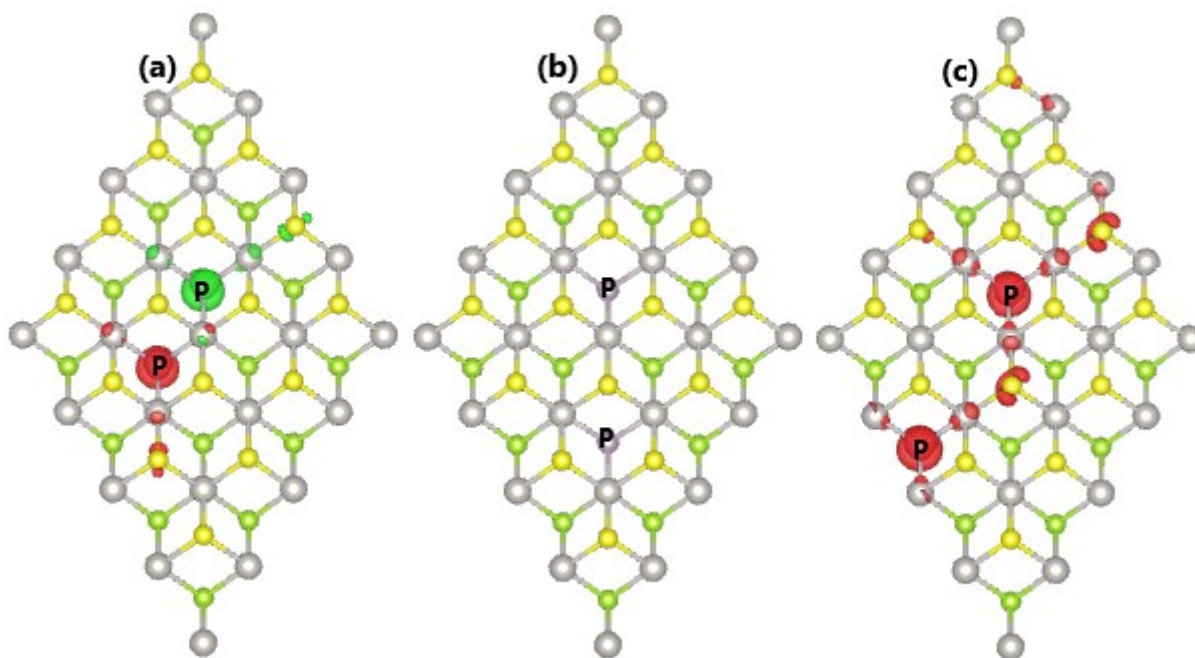


Figure S7: Spin density (Iso-surface value: $0.005 e/\text{\AA}^3$) in (a) Antiferromagnetic, (b) Non-magnetic, and (c) Ferromagnetic 2P-doped PtSSe monolayer.

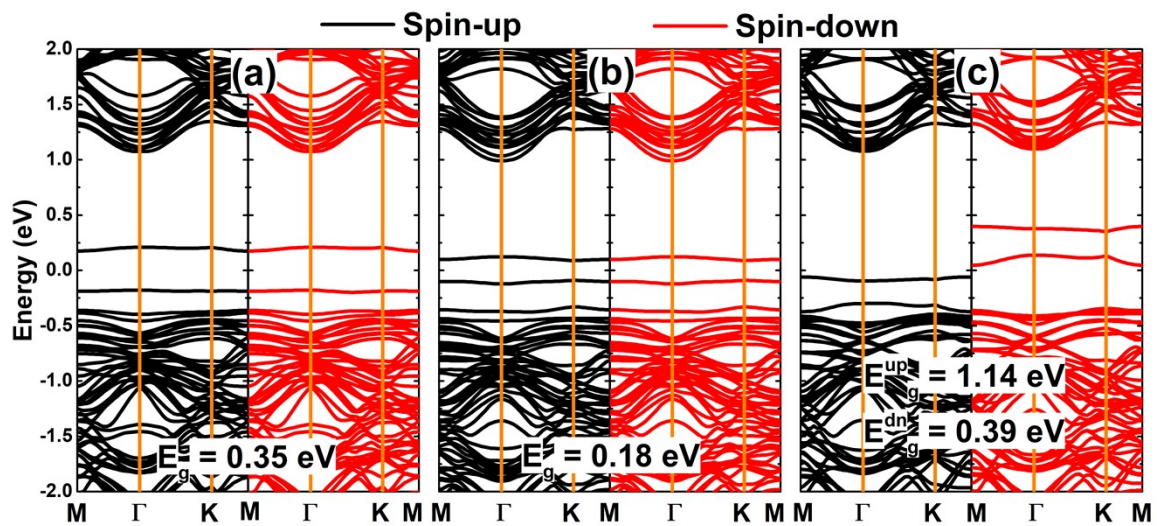


Figure S8: Spin-polarized band structure of (a) Antiferromagnetic, (b) Non-magnetic, and (c) Ferromagnetic 2P-doped PtSse monolayer.