Theoretical insights into PtSSe-SnSSe heterostructures for renewable energy applications

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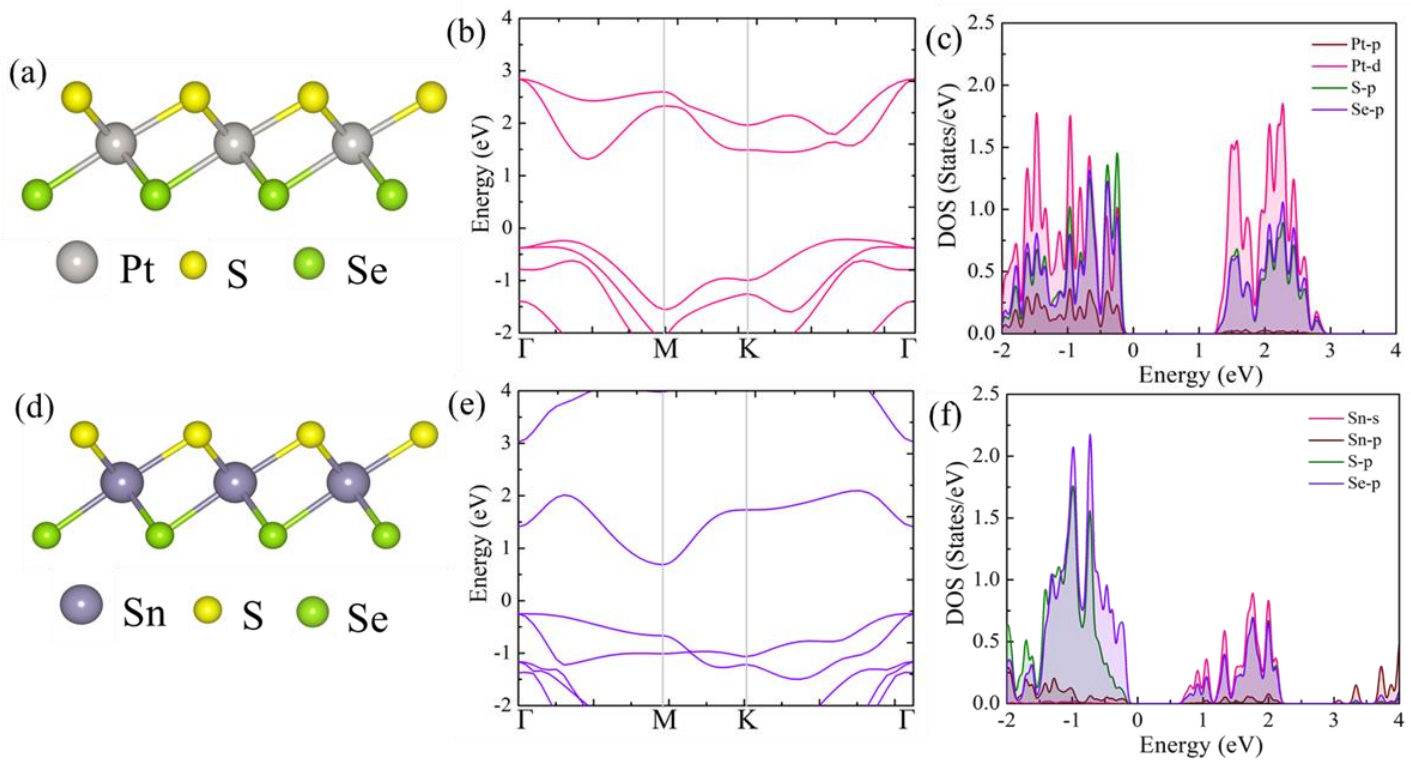
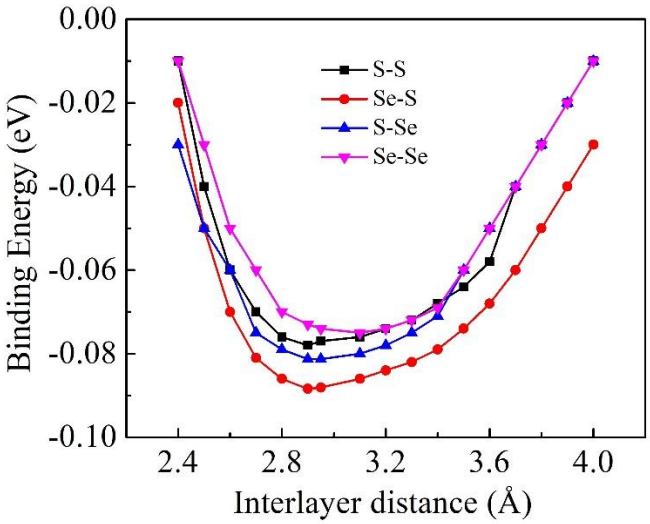
Supplementary Information

STable 1: The optimized lattice constants, bond lengths and bond angles and GGA level band gaps in the PtSSe and SnSSe single layers (SLs)

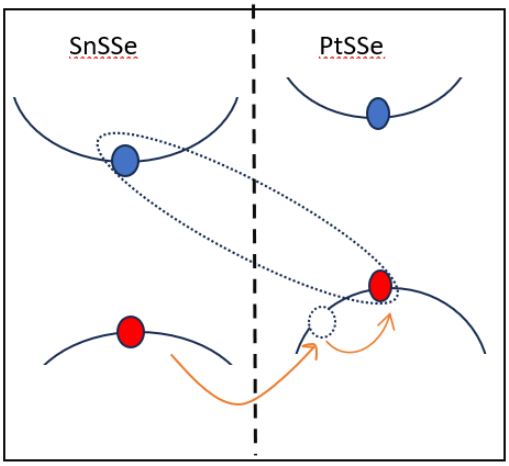
Structure	Lattice constant, a (Å)	Bond length (Å)	Bond angle (degrees)	Band gap (eV)
PtSSe	3.66	Pt-S: 2.43 Pt-Se: 2.50	SPtSe: 84.13	1.52
SnSSe	3.78	Sn-S: 2.62 Sn-Se: 2.72	SSnSe: 89.92	0.94



SFig. 1 The perpendicular views of the structures, electronic band structure and orbital resolved density of states of the single layers (SLs) PtSSe ((a), (b) and (c)) and SnSSe ((d), (e) and (f)). The results shown here are within the GGA.



SFig. 2 The variation in the binding energy with respect to the interlayer distance in the four stacking configurations of the PtSSe-SnSSe vdWHS.



SFig. 3 The charge transfer mechanism in PtSSe-SnSSe vdWHS. The blue and red circles represent electron and hole respectively.