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


**Electronic Supplementary Information for**

# "Theoretically proposed stable polymorph of two-dimensional pentagonal $\beta$-PdPSe"

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The coordinates and lattice parameters of the optimized geometries for $\beta$-PdPSe in the VASP-POSCAR format.

$\beta$-PdPSe
1.0
5.8884139061 0.0000000000 0.0000000000
0.0000000000 5.8375825882 0.0000000000
0.0000000000 0.0000000000 20.0000000000
P Pd Se
4 4 4
Direct
0.396371722 0.115974844 0.513916910
0.896356881 0.364004582 0.513900876
0.396475226 0.116266422 0.627569735
0.896457851 0.364286005 0.627561331
0.028387094 0.997567654 0.493665248
0.528337240 0.482423574 0.493632823
0.028453387 0.997890830 0.647841871
0.528453052 0.482724309 0.647814691
0.142407417 0.604479432 0.462046593
0.642390966 0.875545144 0.462092340
0.142539009 0.604797065 0.679377556
0.642487407 0.875839829 0.679416537

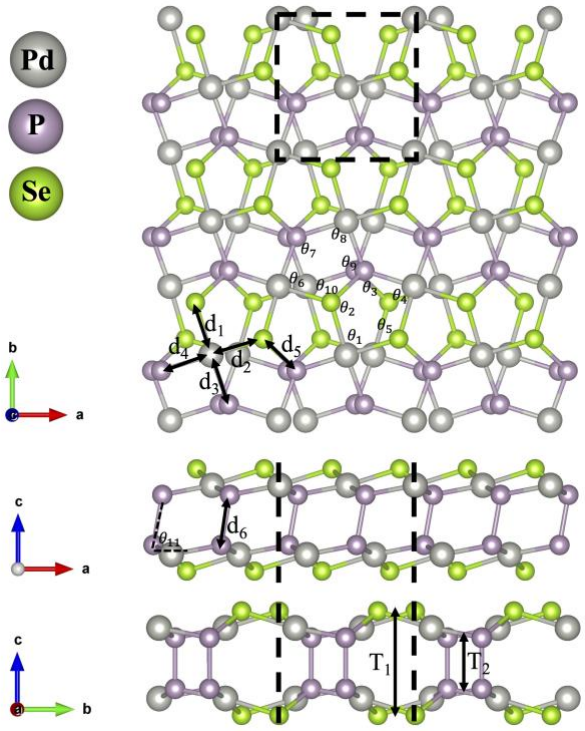


Fig. S1 3x3 supercell of pentagonal $\alpha$-PdPSe geometrical structures.

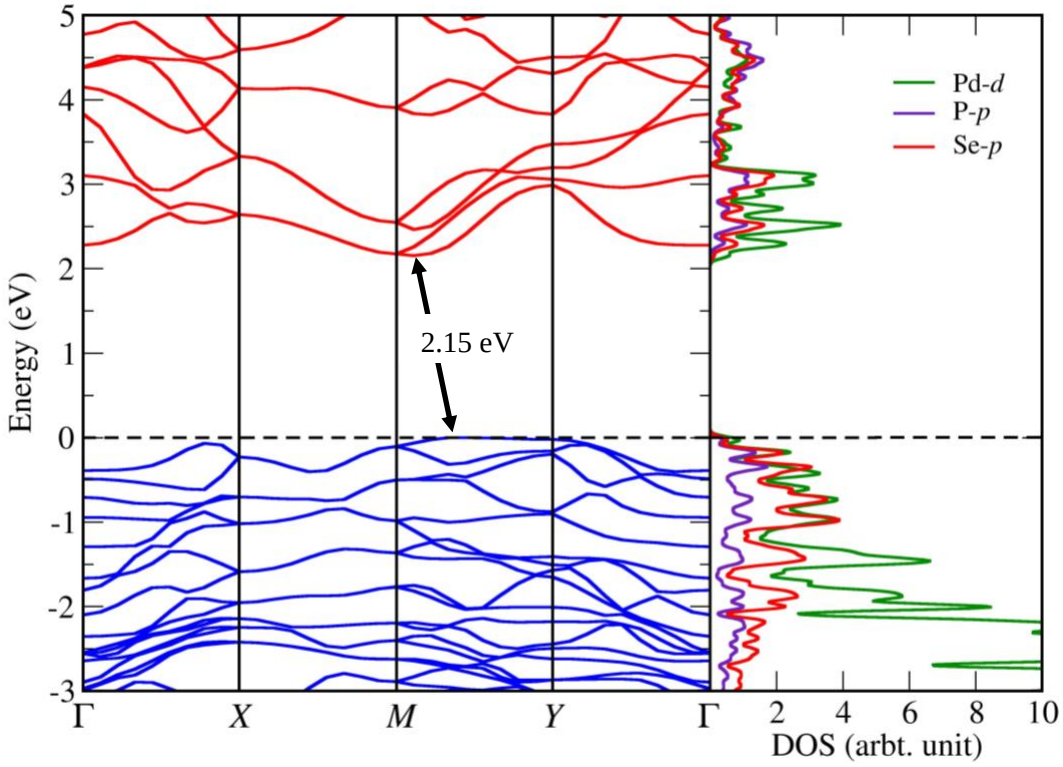


Fig. S2 Calculated band structure and partial density of state (PDOS) for pentagonal $\alpha$-PdPSe.

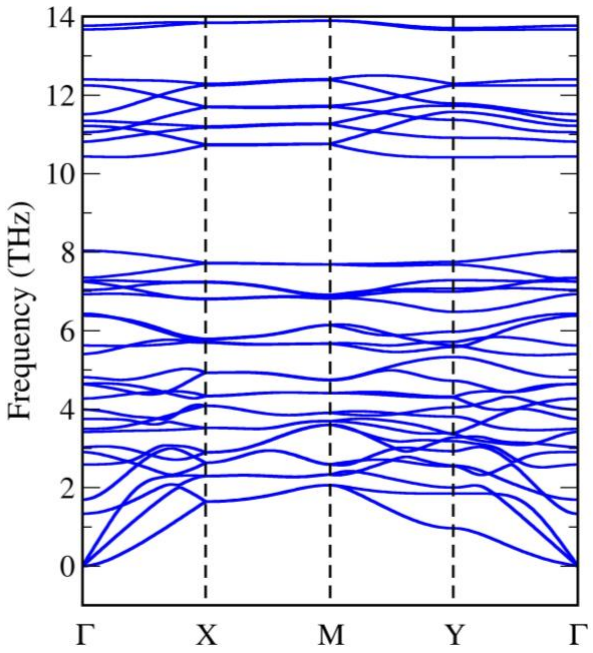


Fig. S3 Calculated phonon band structure of $\alpha$-PdPSe.

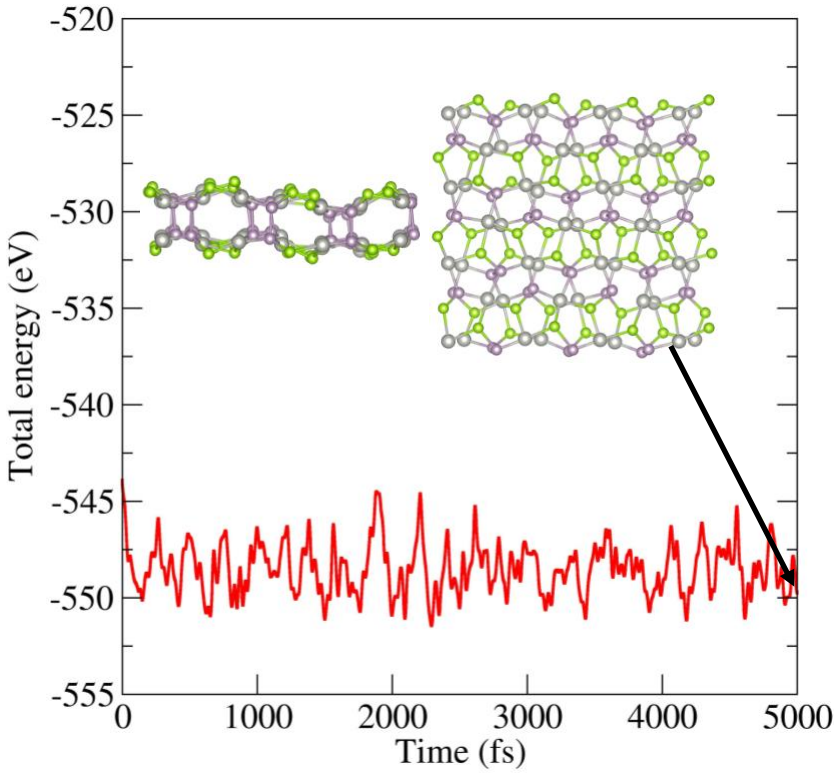


Fig. S4 Total energy fluctuation with time during the AIMD simulation at 1000 K of $\alpha$-PdPSe.

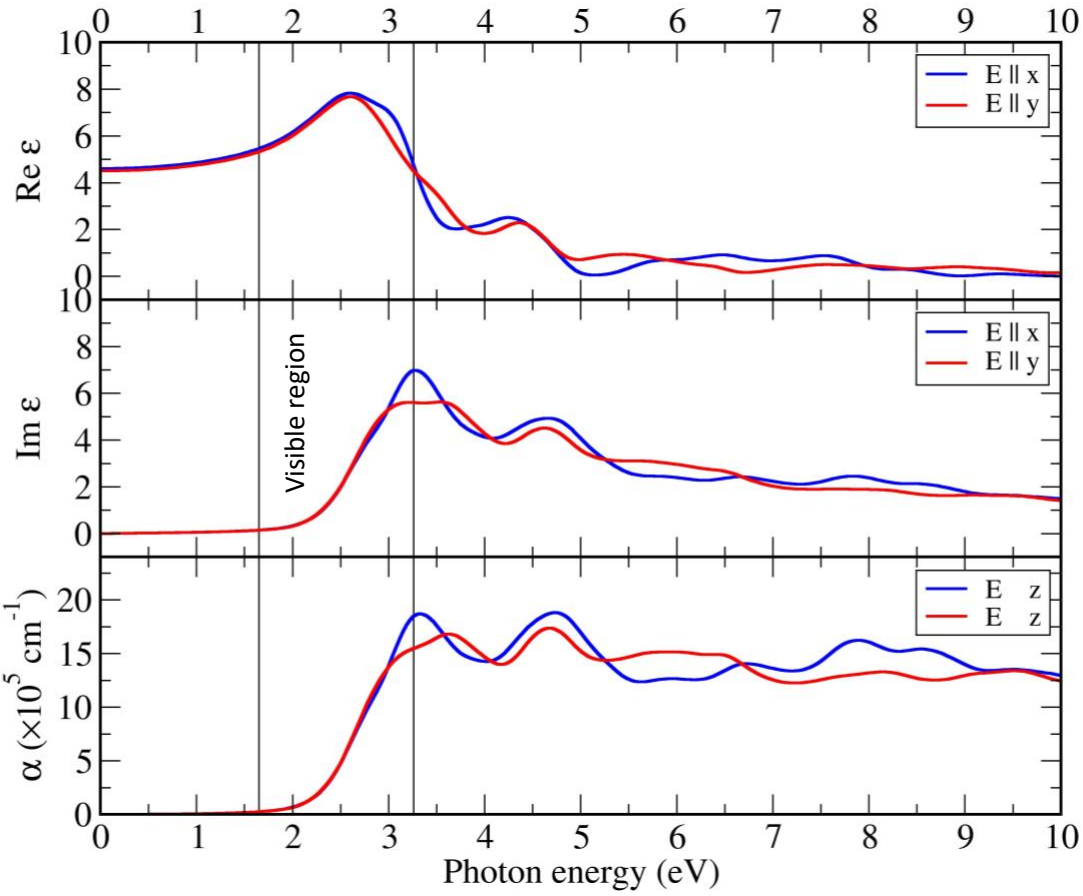


Fig. S5 Real part and Imaginary part of the dielectric function as a function of in-plane photon energy (x- and y-polarized light) for $\alpha$ phase *penta*-PdPSe.