

Supporting Information

Few-layers PdSe₂ sheets: The promising thermoelectric materials driven by high valley convergence

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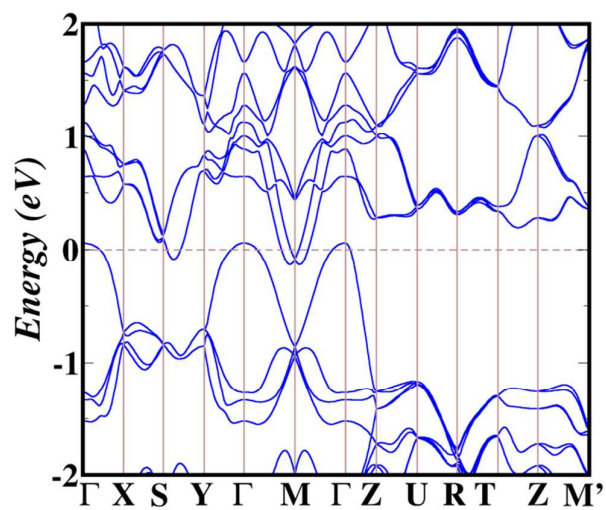


Figure S1. Electronic band structure of bulk PdSe₂ calculated by PBE-TS+SCS+SOC method. The Fermi level has been set to zero and indicated by the dashed line.

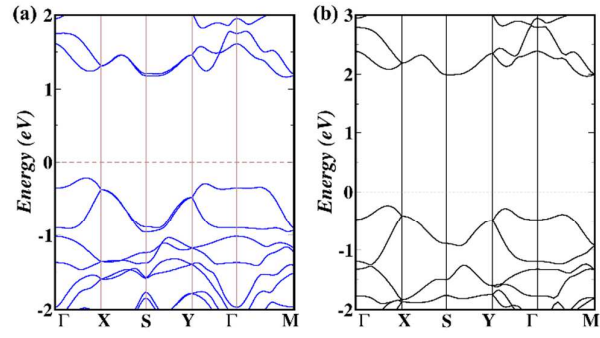


Figure S2. Electronic band structures of monolayer PdSe₂ calculated by the (a) PBE-TS+SCS+SOC and (b) PBE-TS+SCS+HSE06 methods. The Fermi level has been set to zero and indicated by the dashed line.

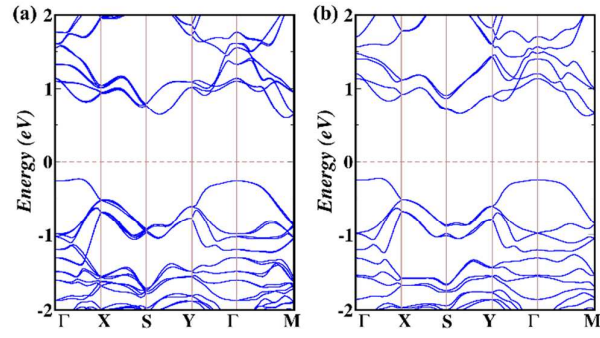


Figure S3. Electronic band structures of bilayer PdSe₂: (a) α -PdSe₂ and (b) β -PdSe₂ calculated by the PBE–TS+SCS+SOC method. The Fermi level has been set to zero and indicated by the dashed line.

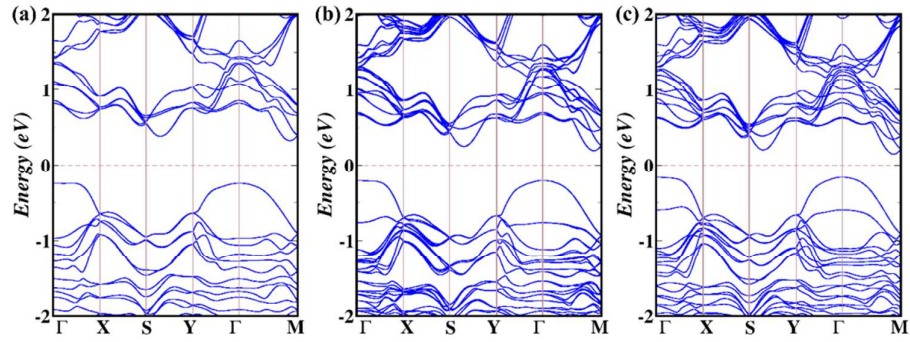


Figure S4. Electronic band structures of (a) trilayer, (b) tetralayer, and (c) pentalayer PdSe₂ calculated by the PBE-TS+SCS+SOC method. The Fermi level has been set to zero and indicated by the dashed line.

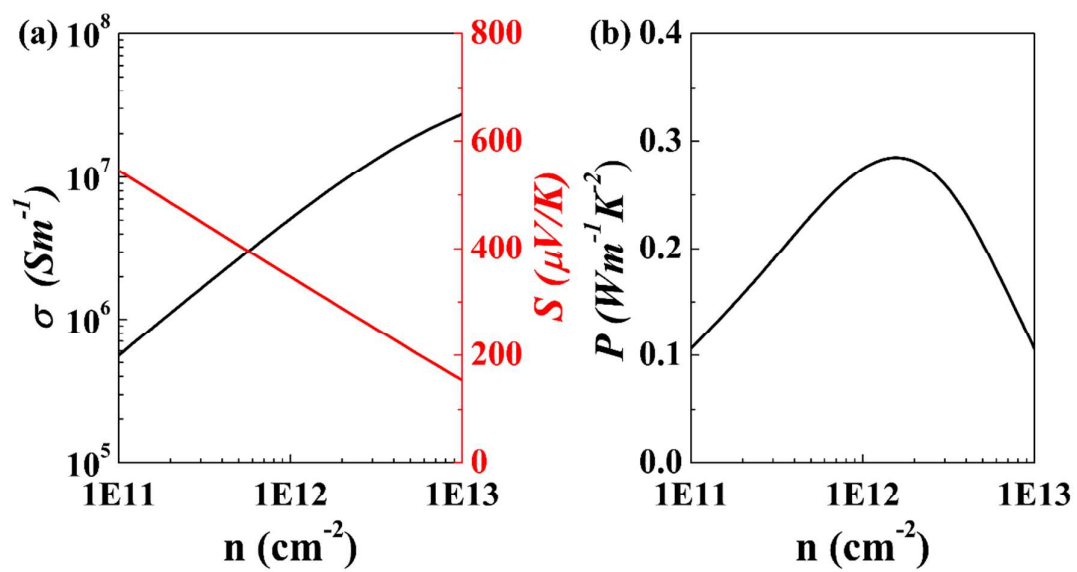


Figure S5. Electronic transport coefficients of monolayer PdSe₂ at room temperature as a function of n . (a) σ and S , and (b) P .

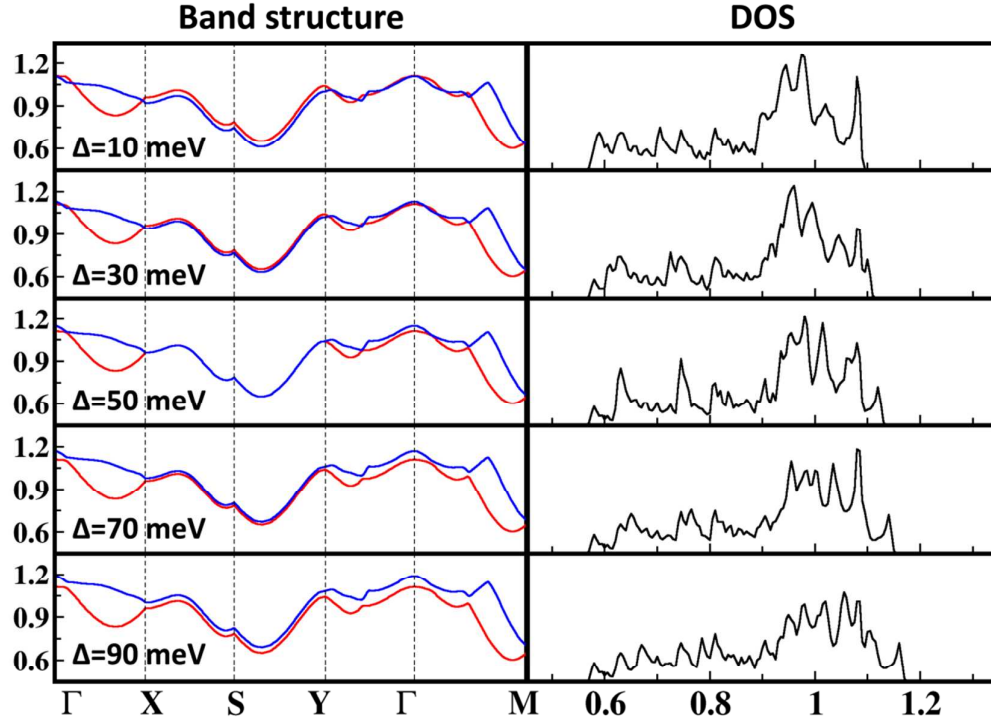


Figure S6. Band structures and PDOSs of the CBM and the CBM+1 states of α -PdSe₂ bilayer with Δ_{CBM} of 10, 30, 50, 70, and 90 meV, respectively.