

Supporting Information

Promising novel thermoelectric materials: Two-dimensional penta-like PtPX (X=S, Se, Te) nanosheets

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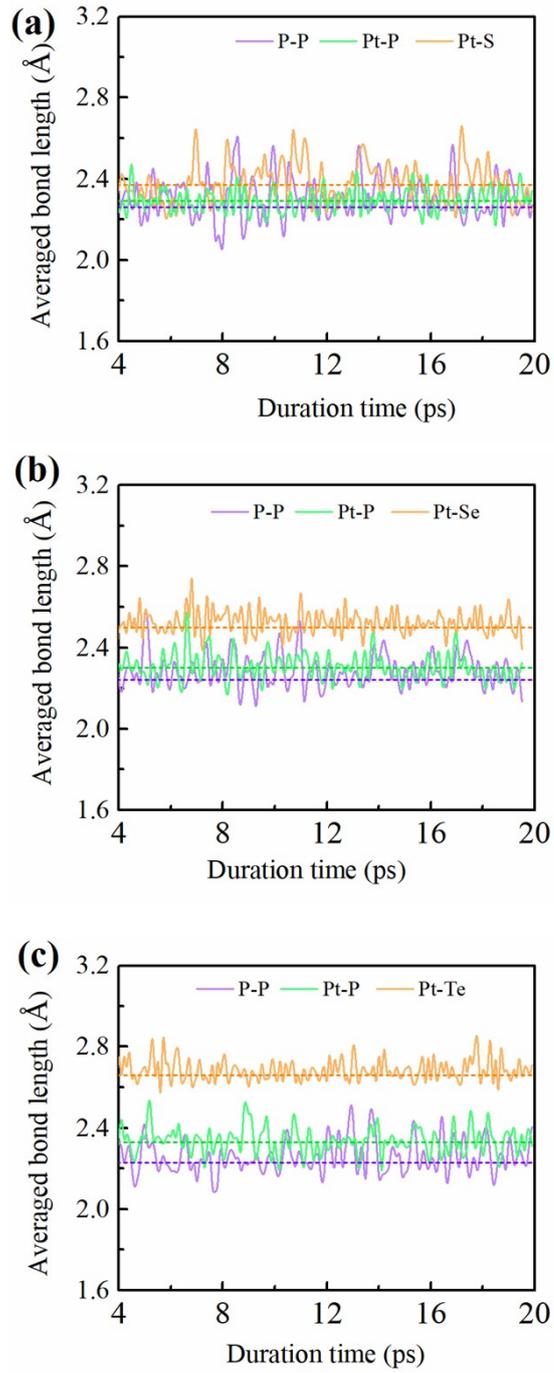


Fig.S1. Bond length of P-P, Pt-P and Pt-X (X=S, Se, Te) as a function of molecular dynamical duration time at 1000 K for (a) PtPS, (b) PtPSe and (c) PtPTe monolayer

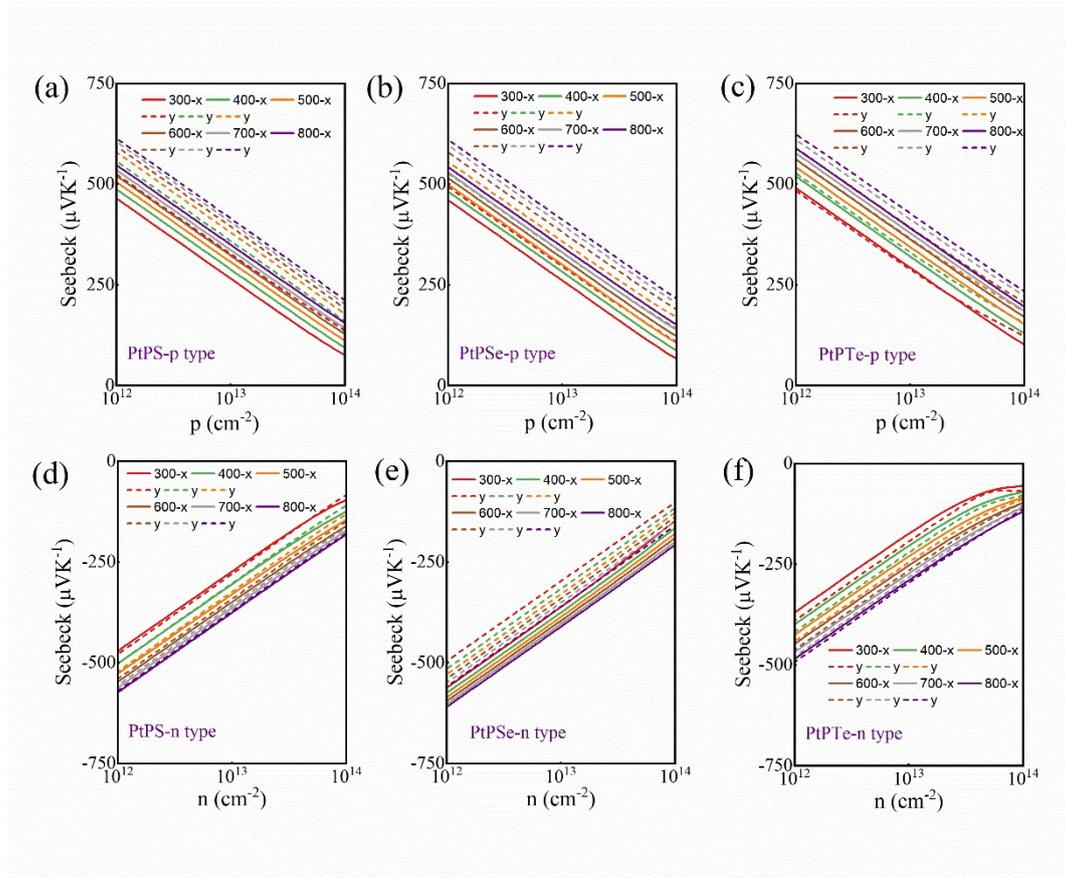


Fig.S2. Seebeck coefficient as a function of carrier concentration for p-type and n-type for (a, d) PtPS, (b, e) PtPSe and (c, f) PtPTE monolayer along x and y directions at different temperature.

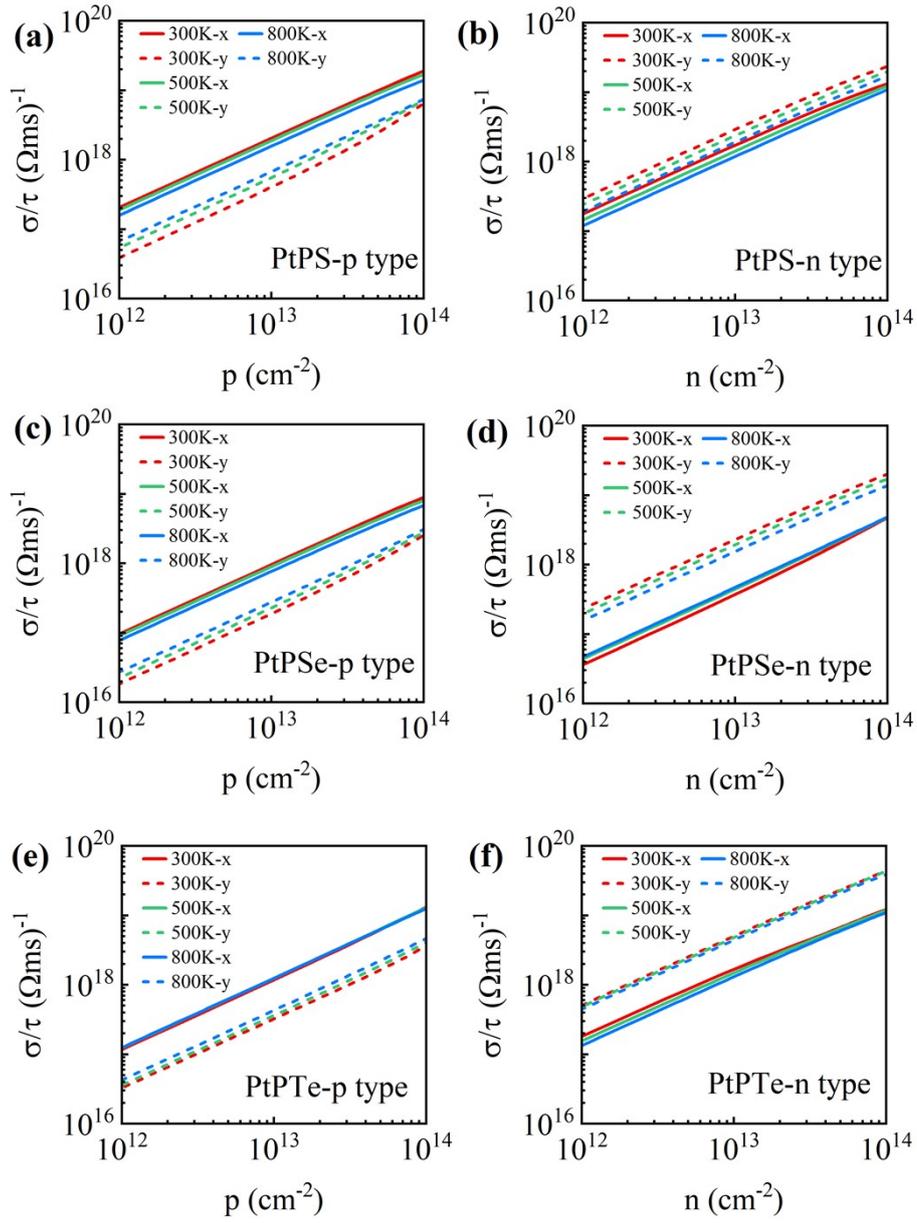


Fig.S3. σ/τ as a function of carrier concentration for p-type and n-type along x and y directions for (a, d) PtPS, (b, e) PtPSe and (c, f) PtPTe monolayer at different temperature.

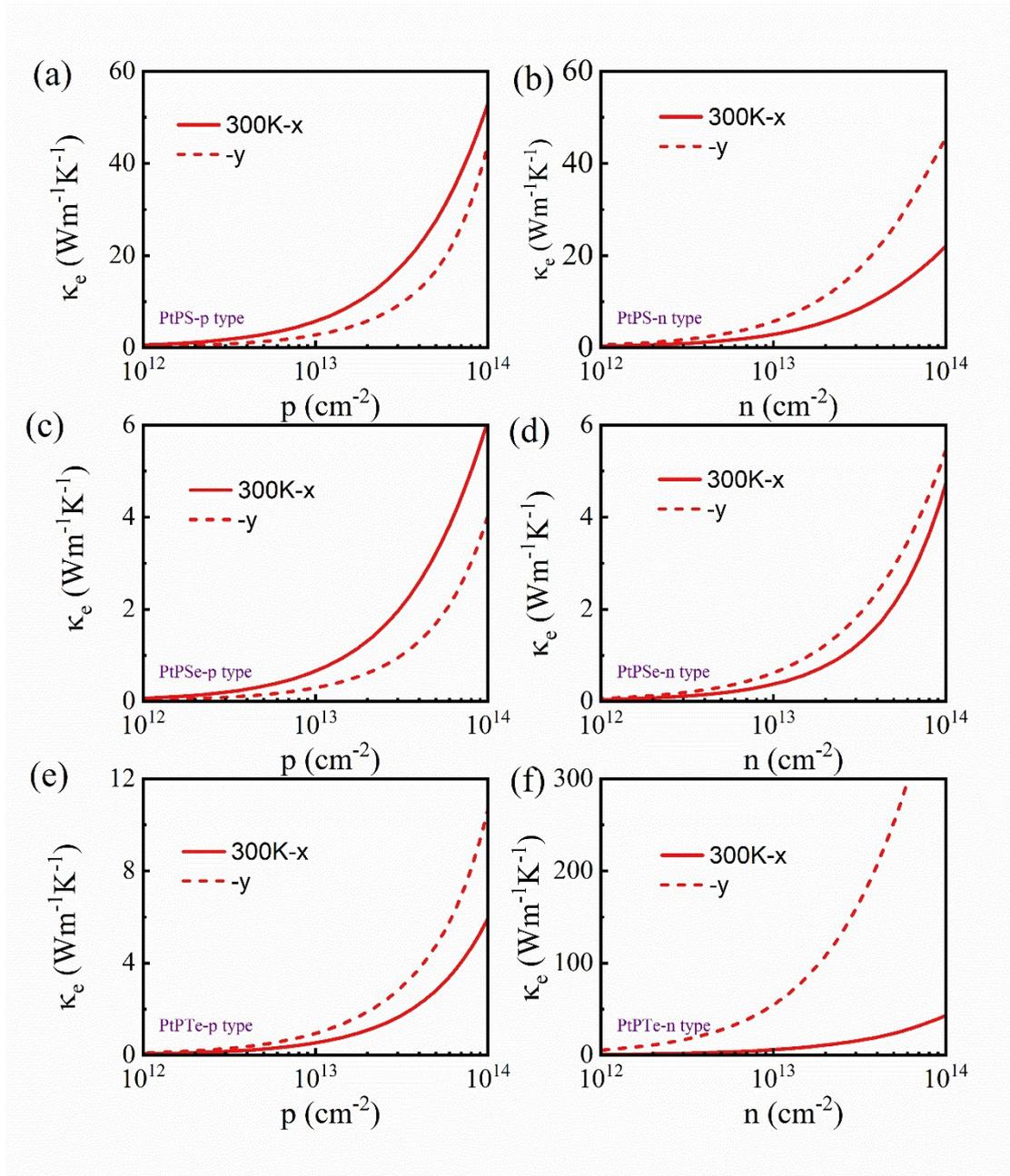


Fig.S4. Electronic thermal conductivity as a function of carrier concentration for p-type and n-type along x and y directions for (a, b) PtPS, (c, d) PtPSe and (e, f) PtPTe monolayer at 300 K.