Supporting Information

1T‴ Transition-Metal Dichalcogenides: Strong Bulk Photovoltaic Effect for Enhanced Solar-Power Harvesting

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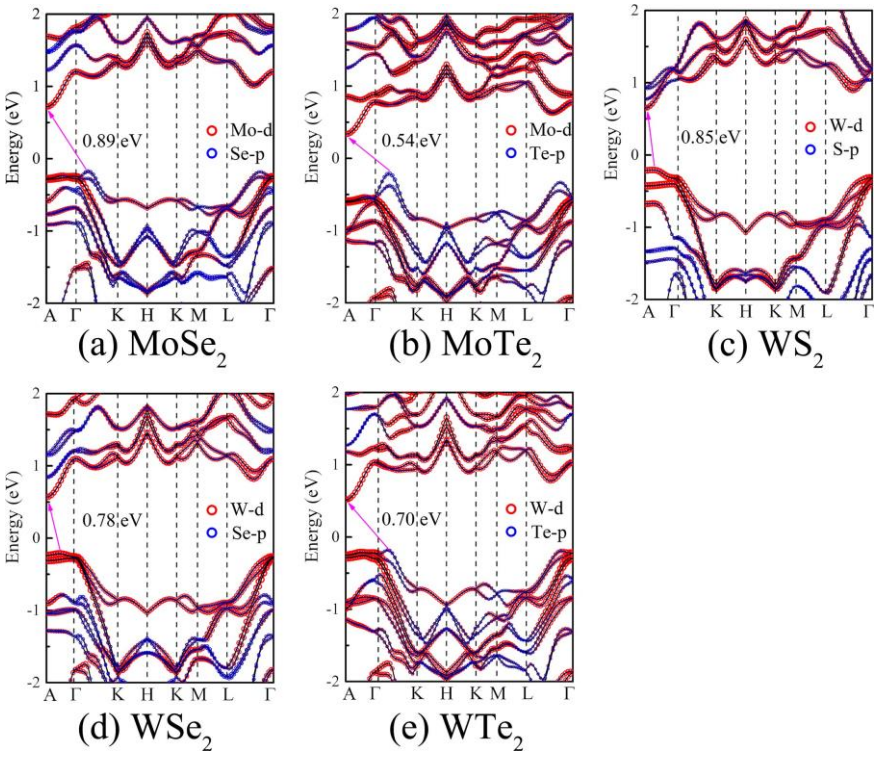

Figure S1. Orbital-resolved band structures based on HSE06 + SOC for 1T‴ bulks: (a) $MoSe_2$, (b) $MoTe_2$, (c) WS_2, (d) WSe_2 and (e) WTe_2. The Fermi level is at 0 eV.

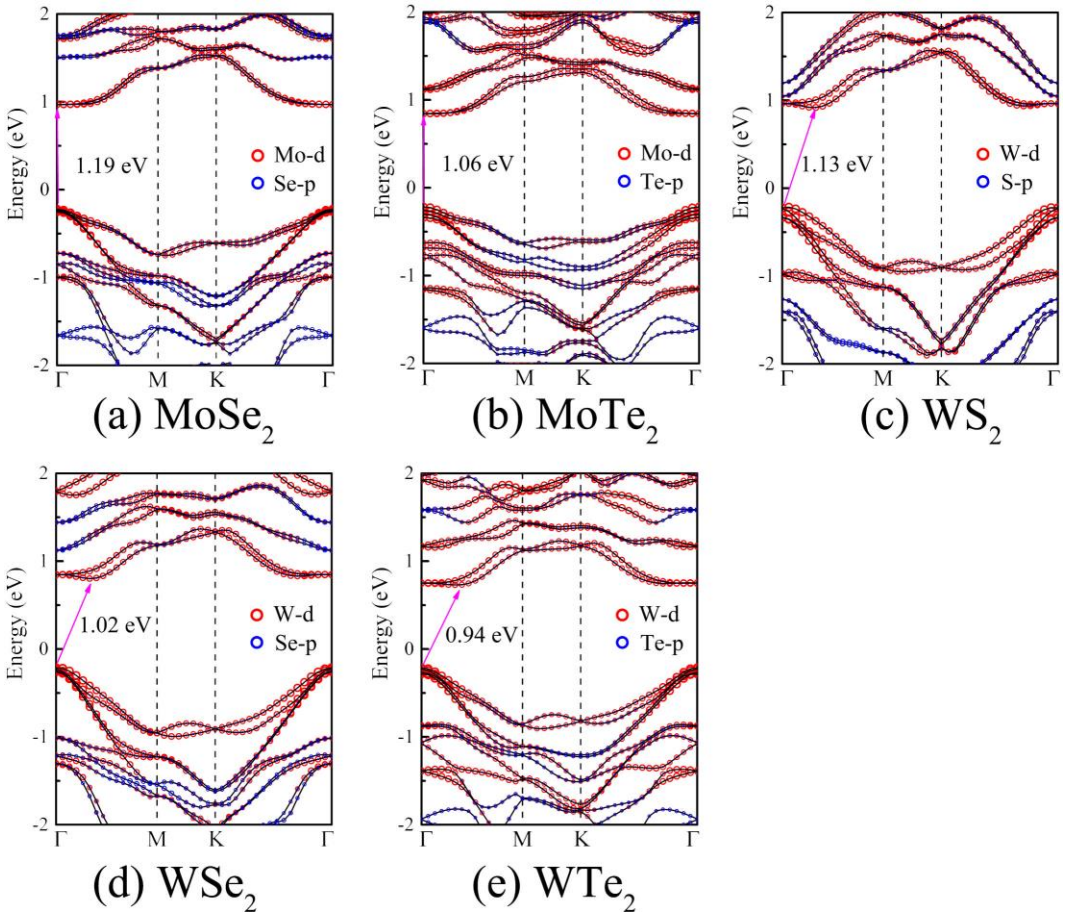

Figure S2. Orbital-resolved band structures based on HSE06 + SOC for 1T‴ monolayers: (a) $MoSe_2$, (b) $MoTe_2$, (c) WS_2, (d) WSe_2 and (e) WTe_2. The Fermi level is at 0 eV.

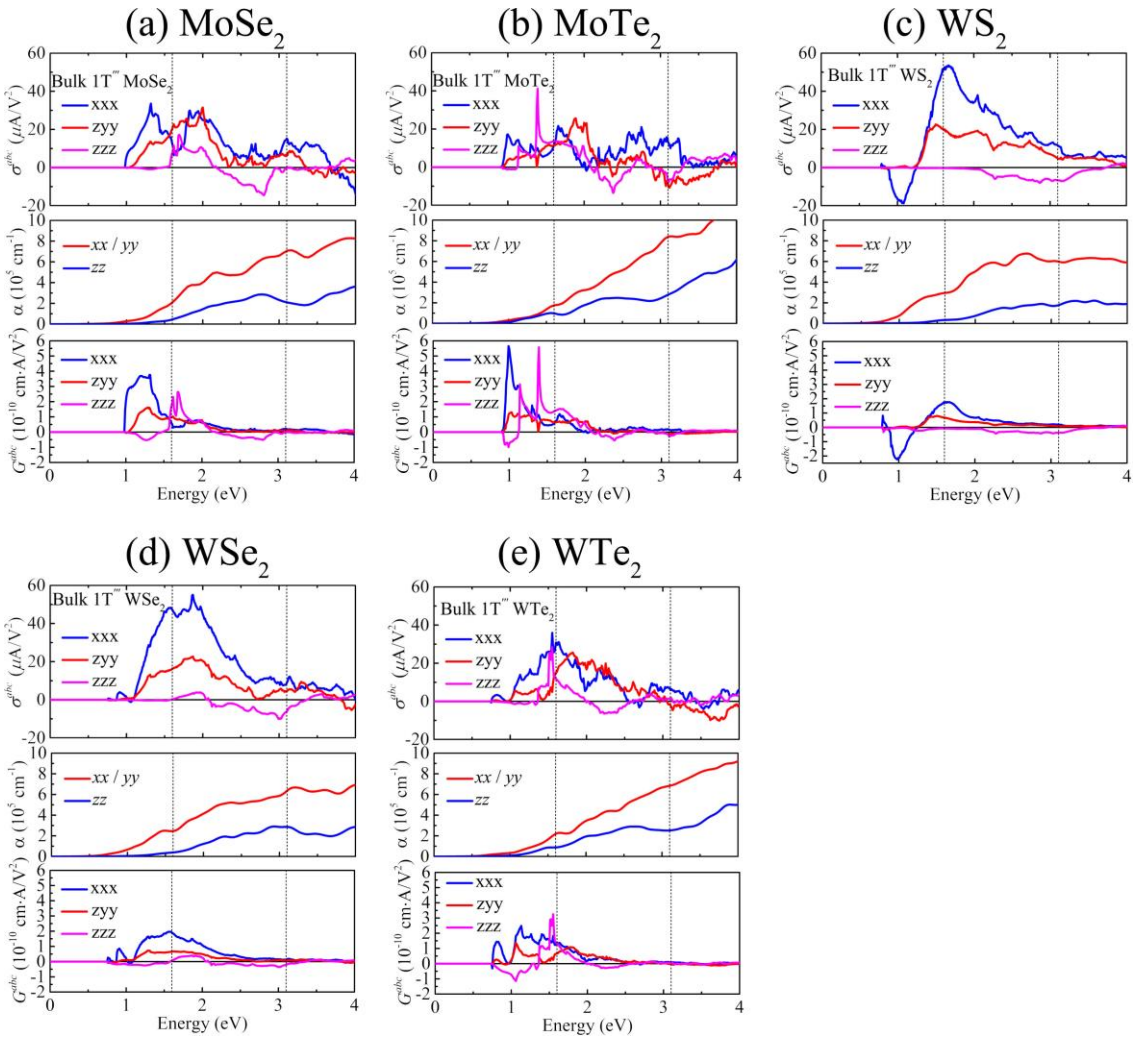

Figure S3. The shift-current responses (σ^{abc}), the optical absorption coefficients (α) and the Glass coefficient responses (G^{abc}) of the 1T‴ bulk (a) $MoSe_2$, (b) $MoTe_2$, (c) WS_2, (d) WSe_2 and (e) WTe_2. The visible light region (1.6–3.1 eV) is within the range of the two dashed lines.

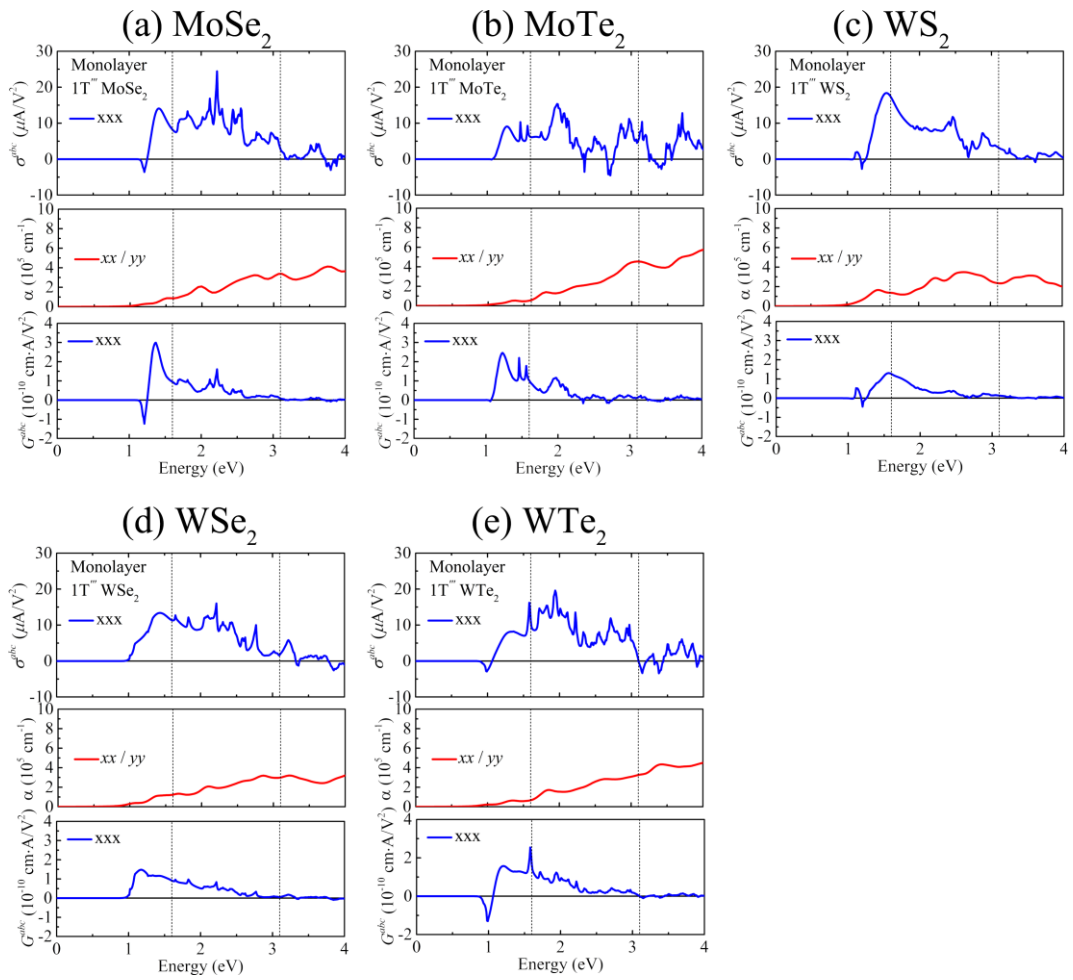

Figure S4. The shift-current responses (σ^{abc}), the optical absorption coefficients (α) and the Glass coefficient responses (G^{abc}) of the 1T‴ monolayer (a) $MoSe_2$, (b) $MoTe_2$, (c) WS_2, (d) WSe_2 and (e) WTe_2. The visible light region (1.6–3.1 eV) is within the range of the two dashed lines.

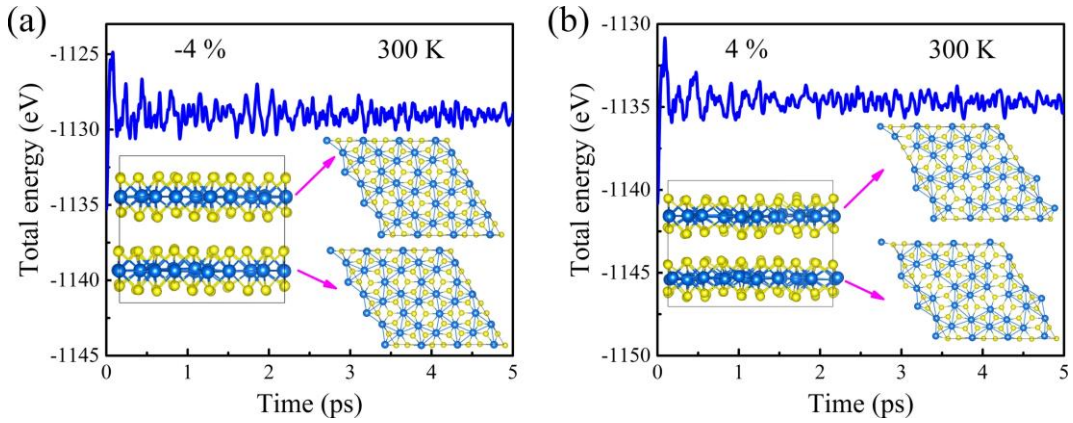

Figure S5. The fluctuation of the total energy of 1T‴-MoS_2-b under the in-plane strain of (a) -4% and (b) 4% during the AIMD simulations at a temperature of 300 K. The insets show the structural snapshots of 1T‴-MoS_2-b at the equilibrium state under 300 K.