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Supplementary Material

Promising transport properties of multifunctional monolayer GeSe nanodevices

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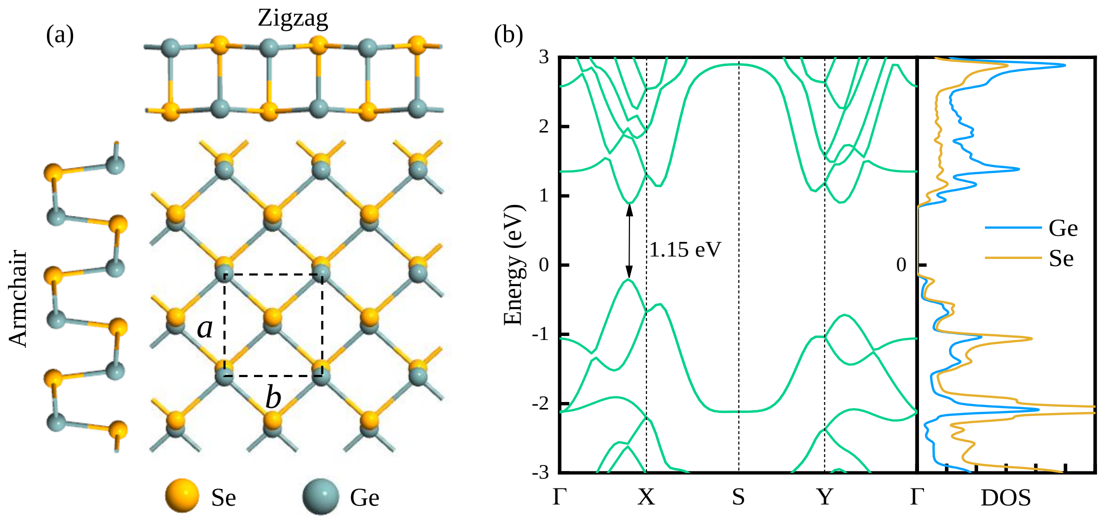

FIG. S1. (a) Top view and side views along the Z-type and A-type directions of ML GeSe, where the black dashed box represents the unit cell. (b) Band structure and DOS of ML GeSe.

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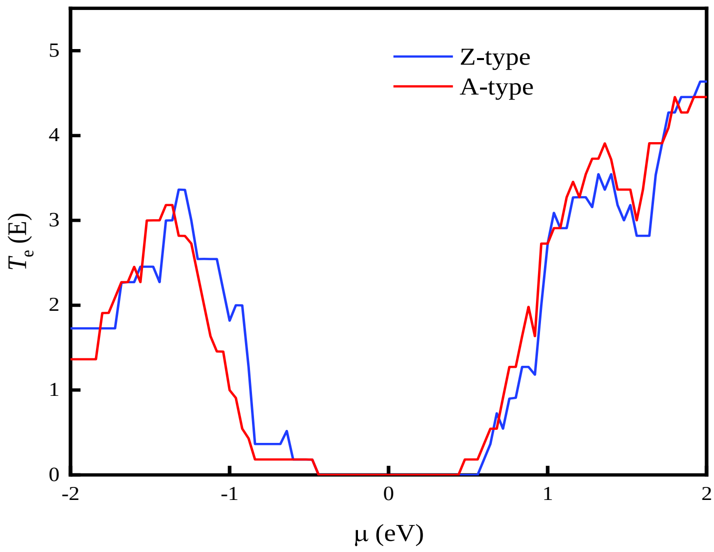

FIG. S2. Electron transmission functions of ML GeSe nanodevices along Z- and A-type directions.

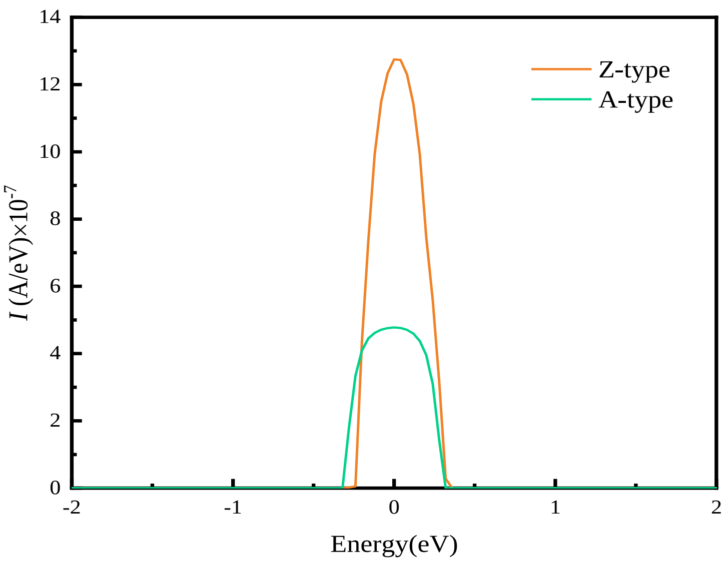

FIG. S3. Spectral current of Z/A-type ML GeSe *p*-*n* junction diode at -0.6 V bias voltage.

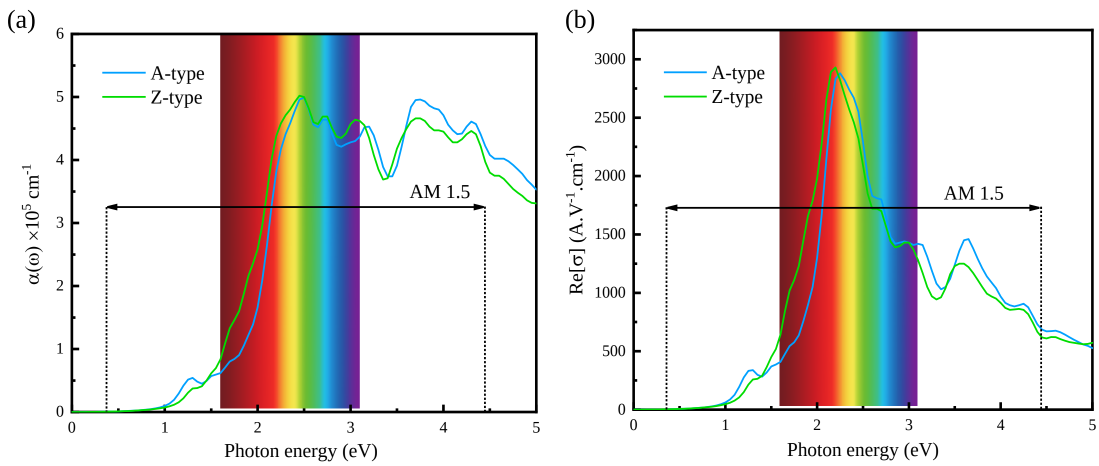

FIG. S4. (a) Optical absorption coefficient $\alpha(\omega)$ and (b) photoconductivity σ of ML GeSe along the in-plane Zigzag (Z-type) and Armchair (A-type) directions.

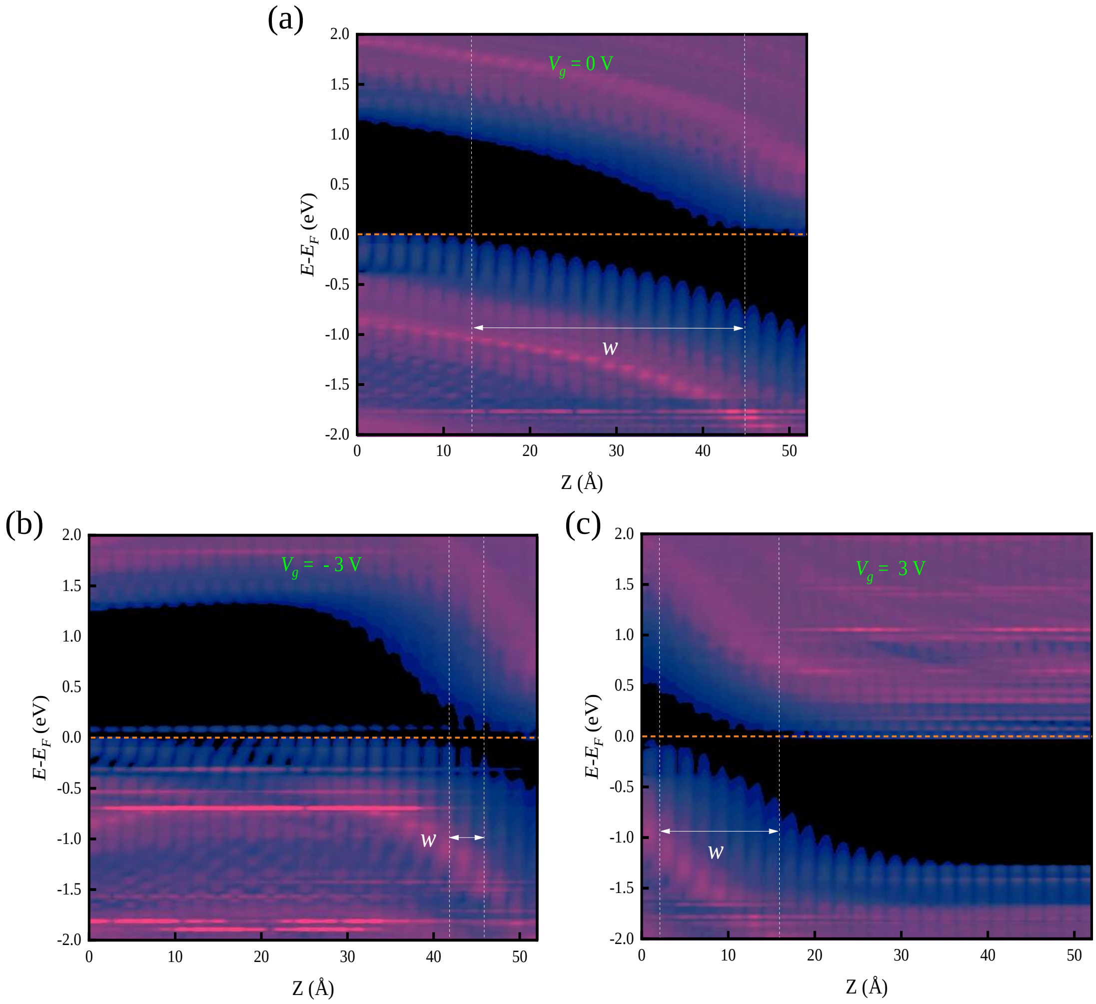

FIG. S5. Projected local density of states (PLDOS) for the Z-type GeSe *p-i-n* homojunction phototransistor at zero bias under 0 V (a), -3 V (b), and 3 V (c) gate voltages, where *w* denotes the width of the depletion region.

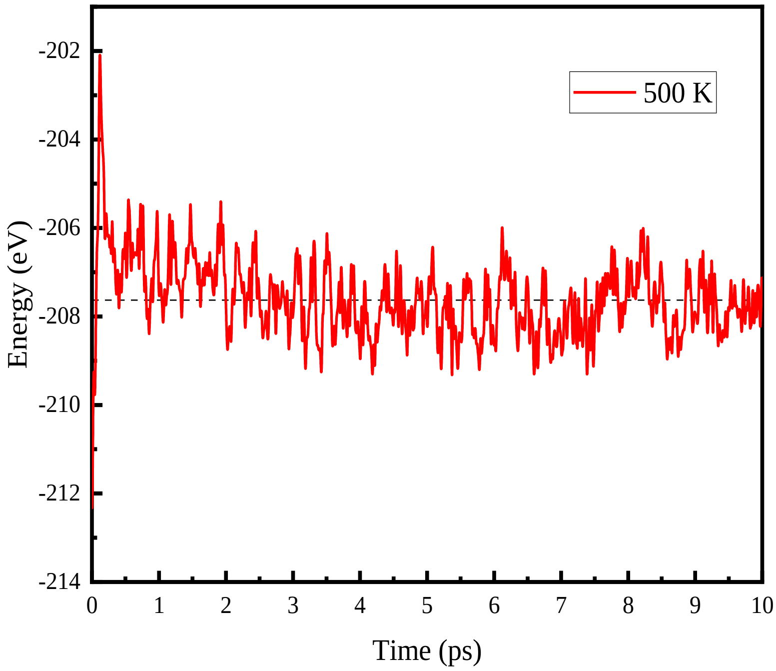

FIG. S6. AIMD simulation of the variation of the total energy of a 4 × 3 × 1 GeSe supercell at 500 K with a time step.

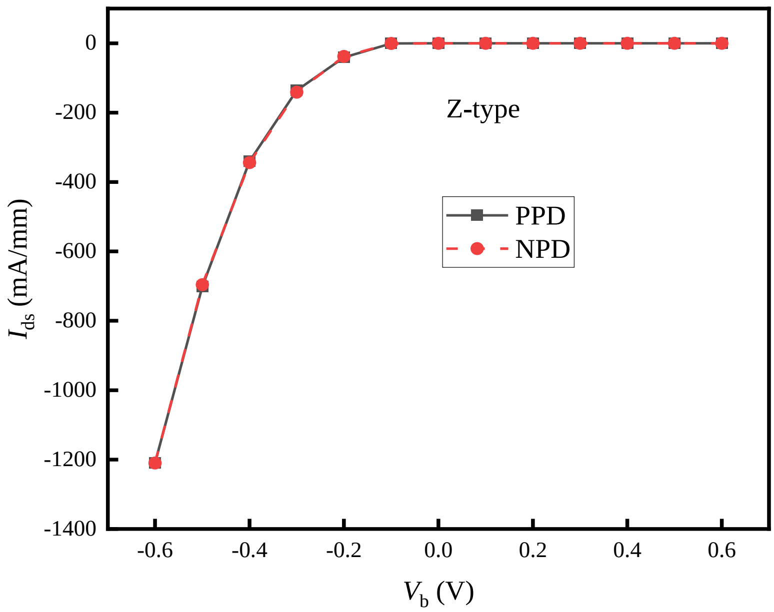

FIG. S7. Current-voltage characteristics of Z-type GeSe *p*-*n* junctions under Periodic, Periodic, and Dirichlet (PPD) and Neumann, Periodic, and Dirichlet (NPD) boundary conditions.

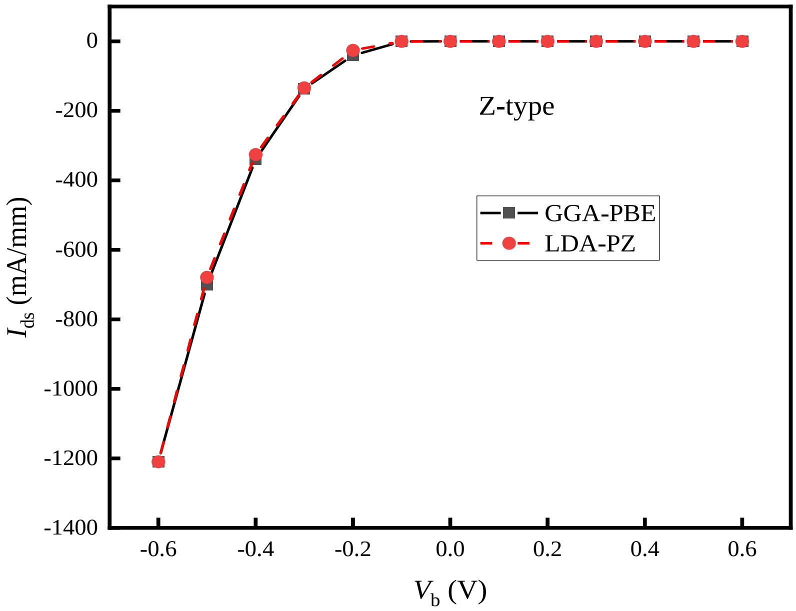

FIG. S8. Current-voltage characteristics of Z-type GeSe *p-n* junctions under GGA-PBE and LDA-PZ exchange-correlation functions.