Supporting Information for "Correlated Roles of Temperature and Dimensionality for Multiple Exciton Generation and Electronic Structures in Quantum Dot Superlattices"

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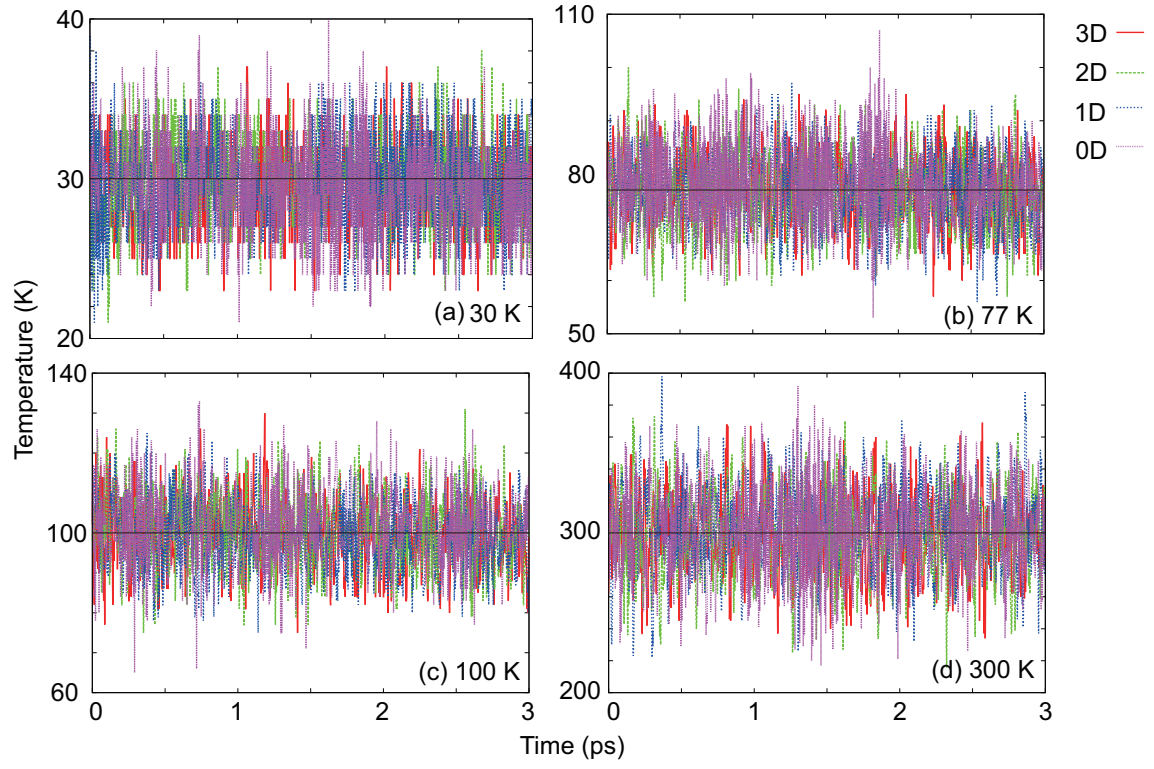
Figure S1: Real-time temperature fluctuations of the $Si_{29}H_{24}$ QDSLs and 0D $Si_{29}H_{24}$ QD at (a) 30 K, (b) 77 K, (c) 100 K and (d) 300 K.
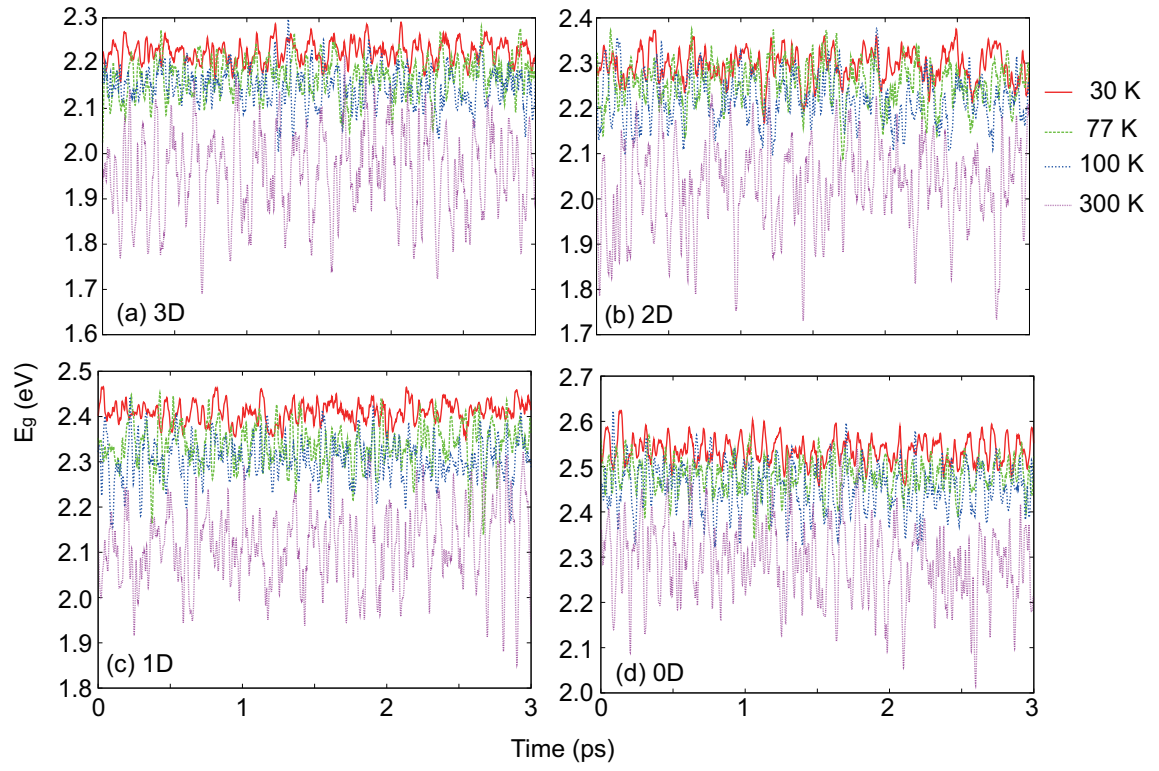
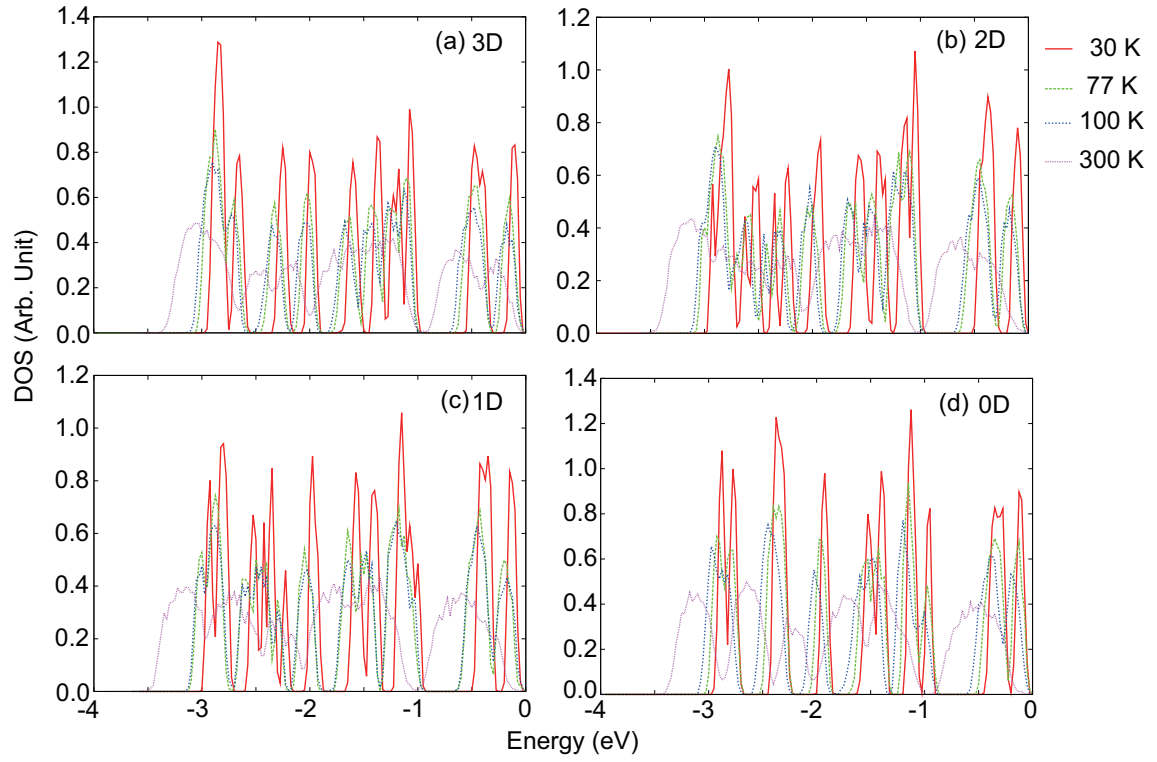Figure S2: Real-time fluctuations of temperature-dependent band-gap energies of the $Si_{29}H_{24}$ QDSLs and 0D $Si_{29}H_{24}$ QD.

Figure S3: VB DOS for (a) 3D, (b) 2D, and (c) 1D $Si_{29}H_{24}$ QDSLs and (d) 0D $Si_{29}H_{24}$ QD. The VB DOS was obtained by counting the number of VB states fluctuating at each temperature along the 3 ps microcanonical MD trajectories. Each highest state was shifted to end with 0 eV for their clear comparison.
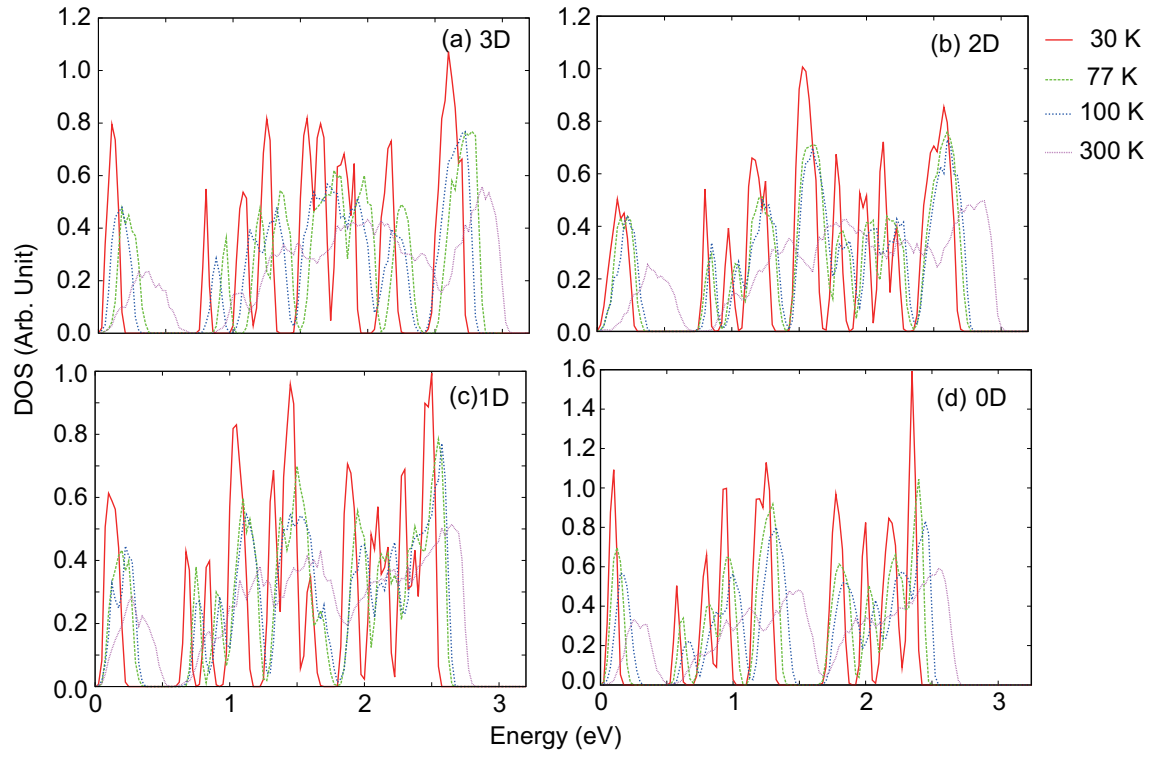
Figure S4: Same as Figure S3 but for the CB states. Each lowest state was shifted to start with 0 eV for their clear comparison.
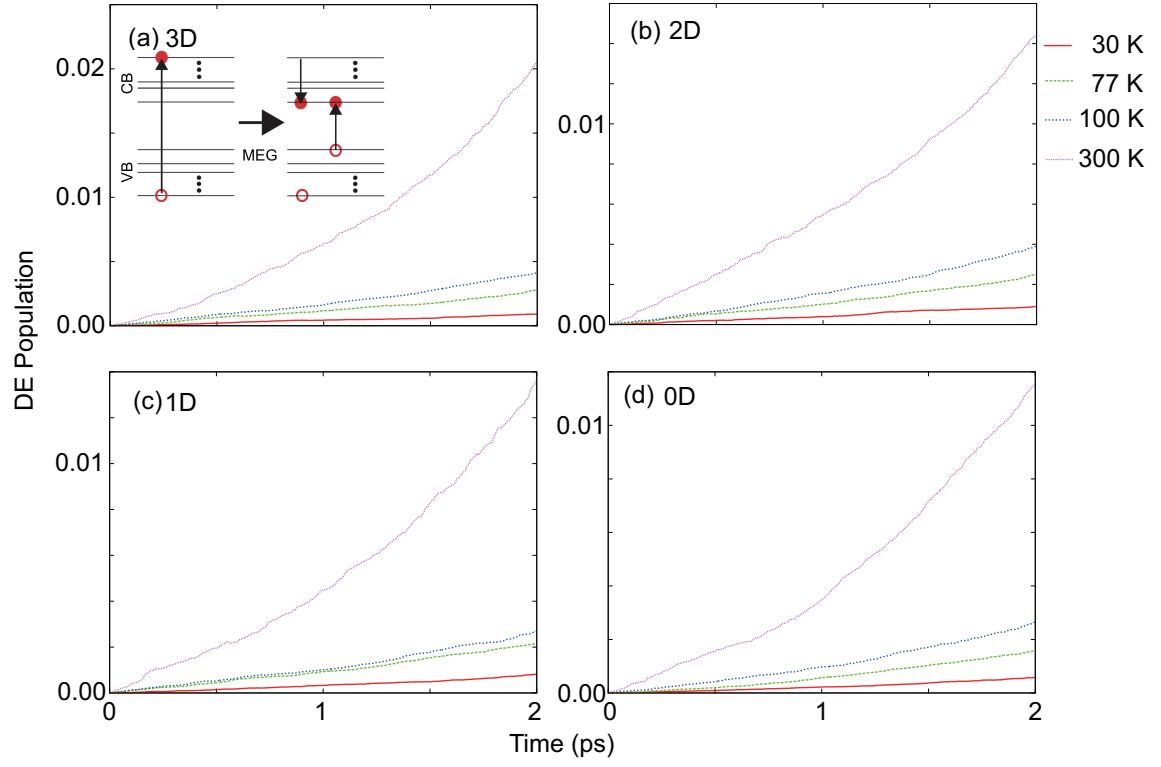
Figure S5: Time-dependent DE population generated through the MEG in (a) 3D, (b) 2D, and (c) 1D $Si_{29}H_{24}$ QDSLs and (d) 0D $Si_{29}H_{24}$ QD.