Electronic Supplementary Information

Heat capacity model of $T^{3/2}$ dependence for quantum confined structures

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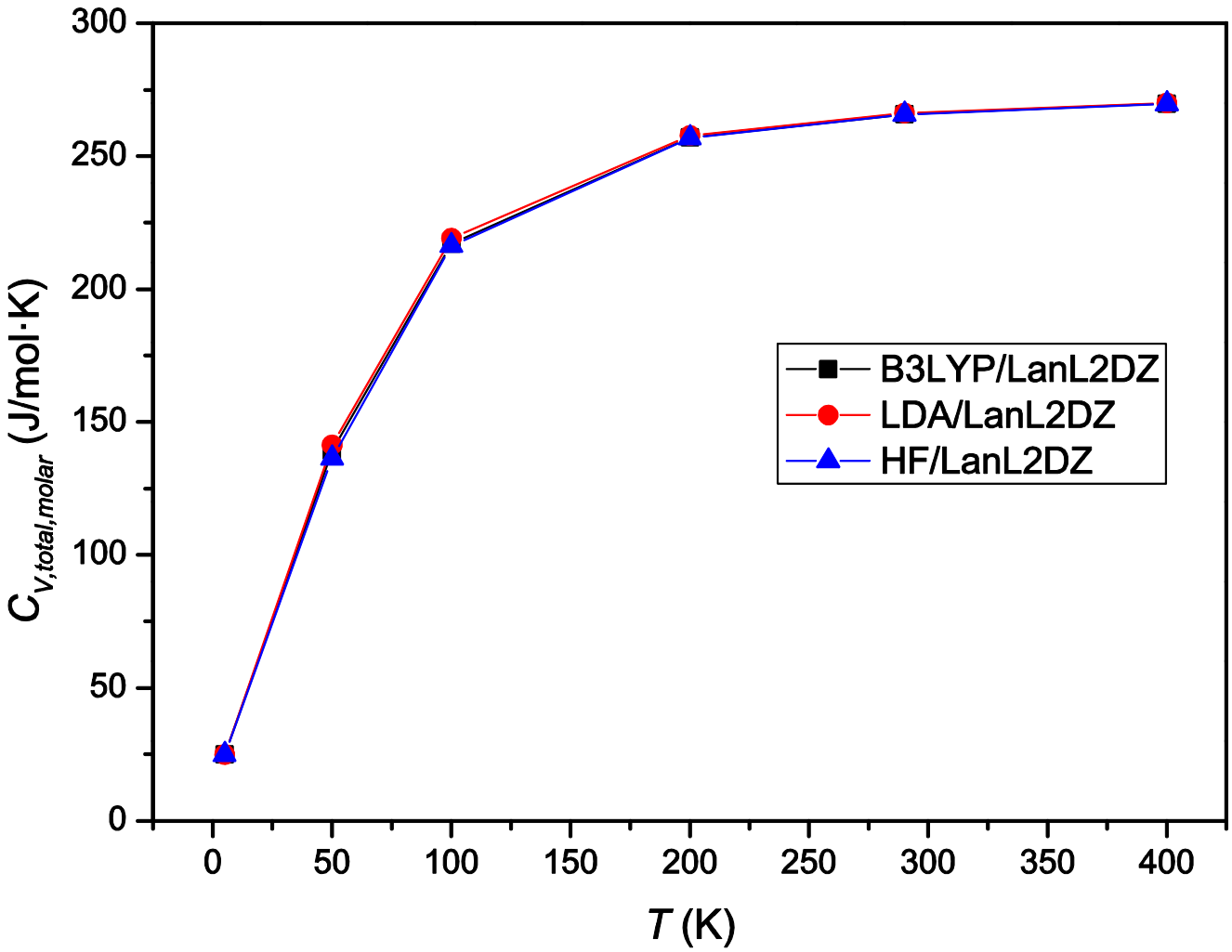
S1. Comparison of thermochemical calculations of $C_{V,total,molar}$ for $(CdSe)_6$ QD cluster at 5, 50, 100, 200, 290, and 400 K using B3LYP/LanL2DZ, HF/LanL2DZ, and LDA/LanL2DZ level of theories

		HF/LanL2DZ		LDA/LanL2DZ	
Temperature (K)	$C_{V,total,molar}$ (J/mol·K) from B3LYP/LanL2DZ	$C_{V,total,molar}$ (J/mol·K)	Percentage of difference (%)	$C_{V,total,molar}$ (J/mol·K)	Percentage of difference (%)
5	24.95756	24.94501	0.05029	24.95338	0.01676
50	139.32302	136.43187	2.07514	141.40665	1.49554
100	217.18307	216.37138	0.37374	219.23742	0.94590
200	257.10680	256.91852	0.07323	257.89758	0.30757
290	265.85554	265.76768	0.03305	266.26139	0.15266
400	269.82616	269.78014	0.01706	270.04791	0.08218



S2. Variation of thermochemical calculations of $C_{V,total,molar}$ for $(CdSe)_6$ QD cluster at 5, 50, 100, 200, 290, and 400 K using B3LYP/LanL2DZ, HF/LanL2DZ, and LDA/LanL2DZ level of theories.