Electronic Supplementary Information:

One-dimensional cadmium sulphide nanotube for photocatalytic water splitting

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Table S1 The computed results obtained by PBE+D2 and HSE06+D2 for planar CdS monolayer and nanotubes. (Lattice parameters a (in Å), Cd−S bond length l (in Å) and total energy E_{tot} (in eV) of planar CdS monolayer. Diameter D (in Å), lattice parameters c_0 (in Å), Cd−S bond length l (in Å) (the value in parentheses is the standard deviation), wall thickness d (in Å) and total energy E_{tot} (in eV) of (3, 0) and (3, 3) CSNTs, respectively.)

Planar	*a*		*l*		E_{tot}
PBE+D2	4.260		2.460 (± 0.000)		-5.980
HSE06+D2	4.260		2.460 (± 0.000)		-5.980
(3, 0) NT	*D*	c_o	*l*	*d*	E_{tot}
PBE+D2	5.186	6.684	2.510 (± 0.007)	0.623	-36.421
HSE06+D2	5.129	6.636	2.491 (± 0.007)	0.580	-36.420
(3, 3) NT	*D*	c_o	*l*	*d*	E_{tot}
PBE+D2	7.739	4.128	2.483 (± 0.010)	0.557	-36.679
HSE06+D2	7.642	4.128	2.466 (± 0.008)	0.510	-36.662

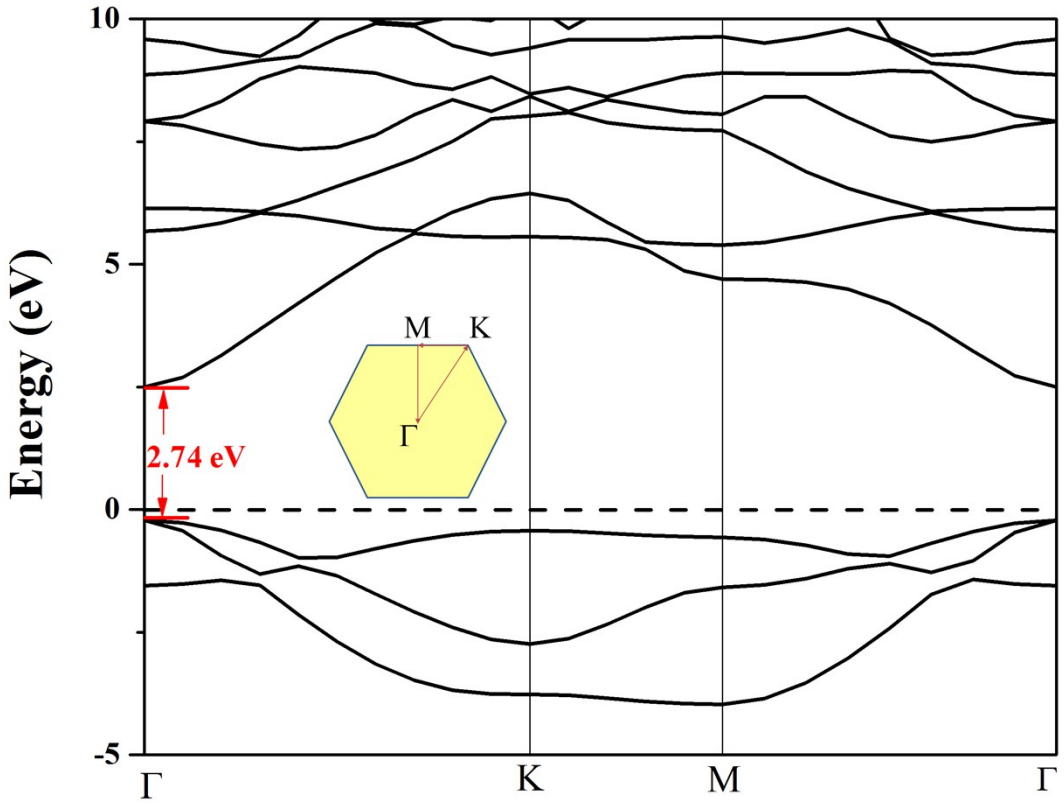

Fig. S1 The calculated band structure of the CdS planar monolayer using HSE06 +D2. The insert is the Brillouin zone.

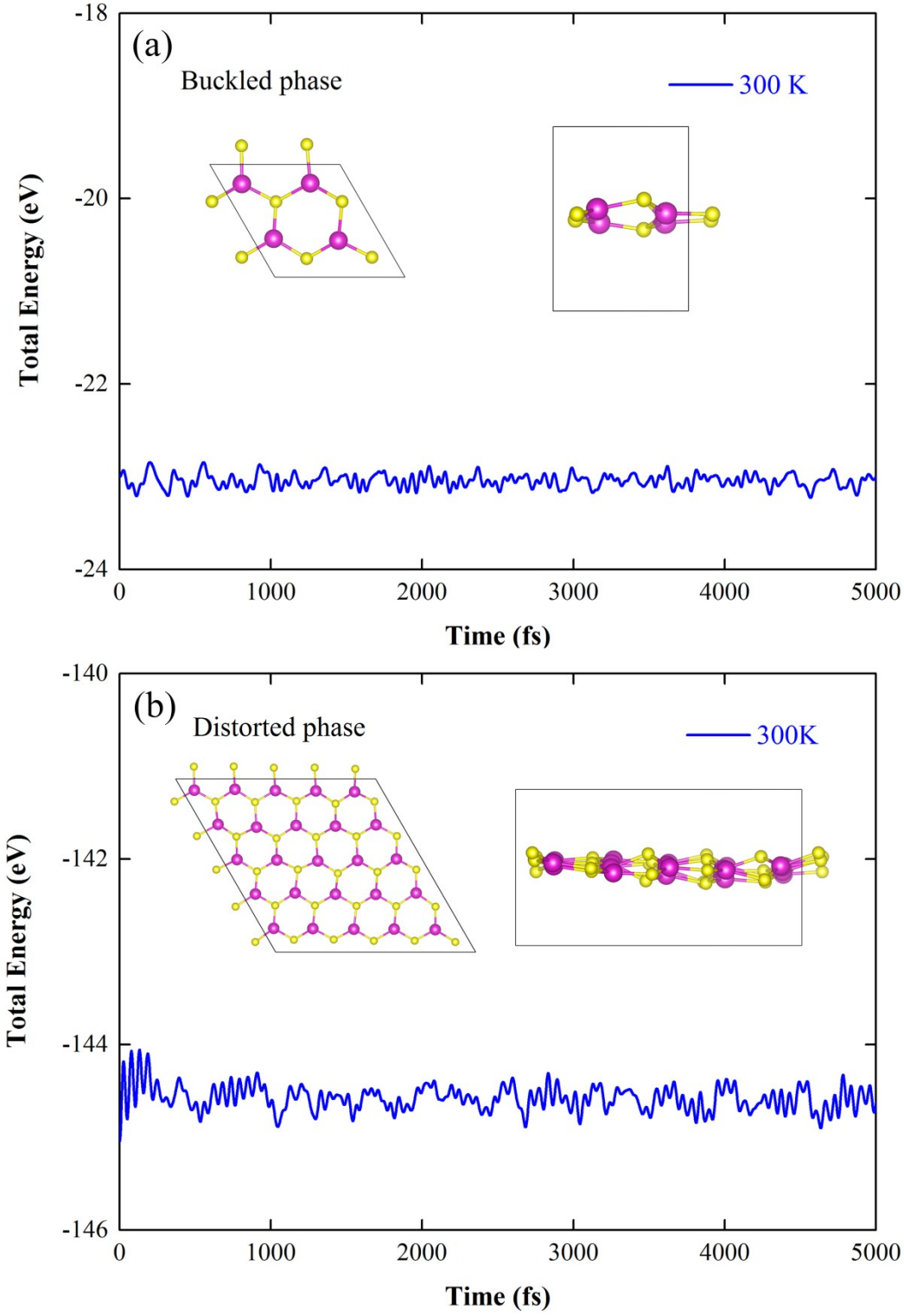

Fig. S2 AIMD simulations of (a) 2 × 2and (b) 5 × 5 CdS monolayer sheet for 5 ps (5000 fs) with a time step of 1 fs at 300 K.

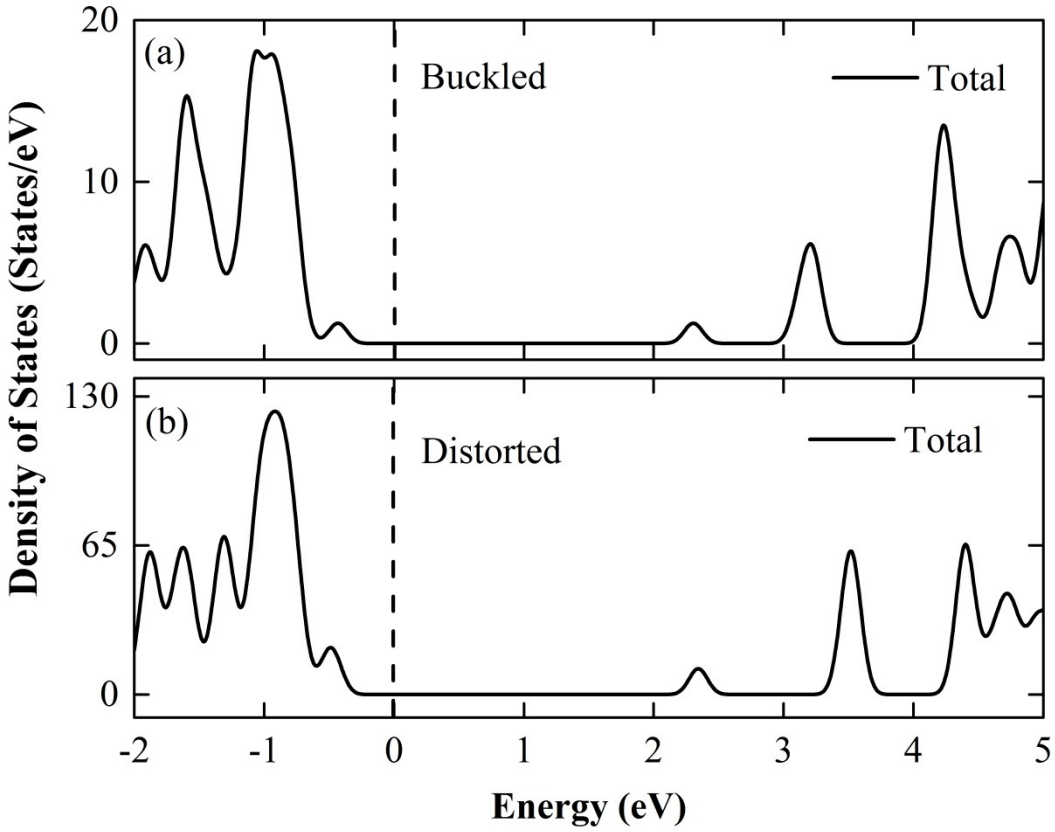

Fig. S3 The calculated total DOS of CdS buckled (a) and distorted (b) monolayer using HSE06+D2.

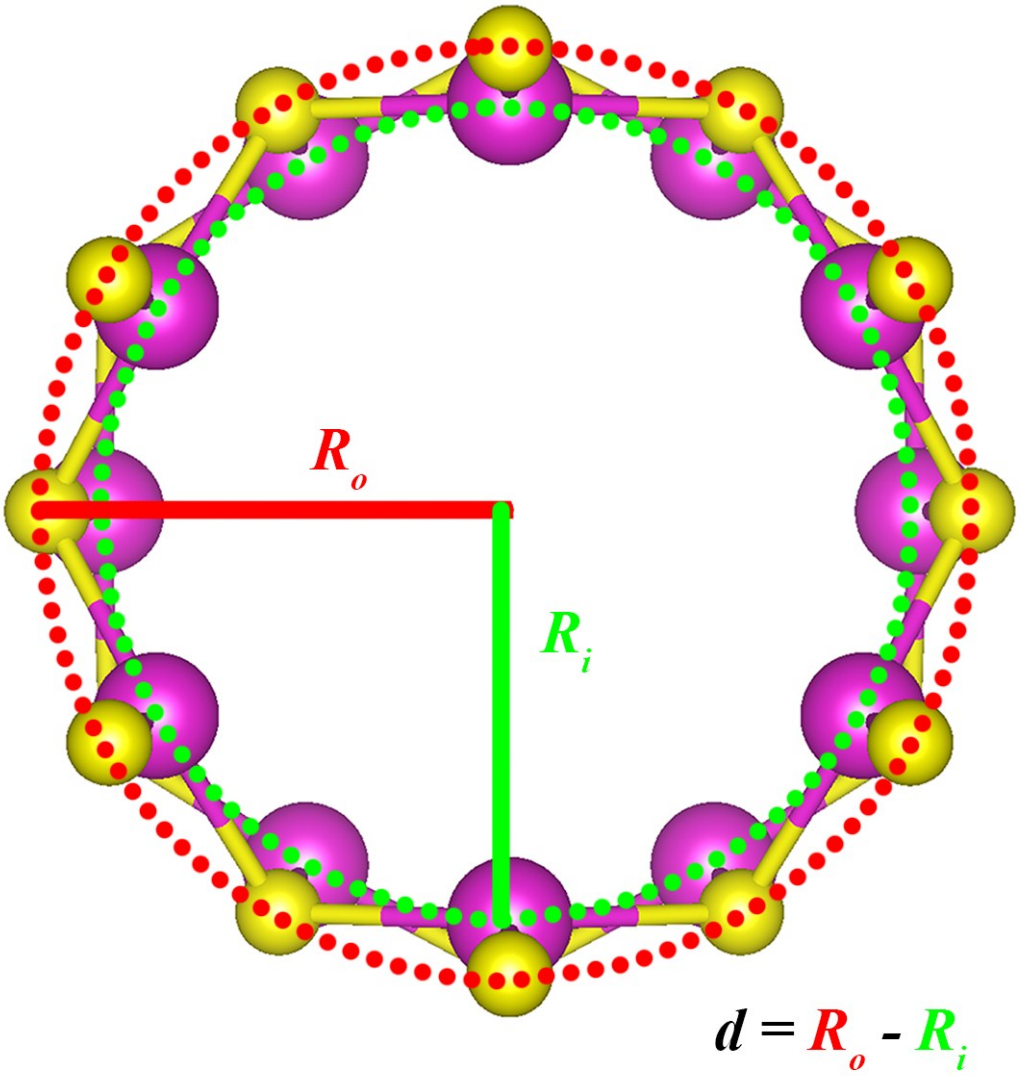

Fig. S4 Top view of the (8, 0) CSNT. The yellow and purple spheres represent S and Cd atoms, respectively. The thickness ($d = R_o - R_i$, R_o and R_i are the outside and inside radius of the CSNTs, respectively) is to identify the corrugation of the CSNT.

Table S2 Effective masses of electrons and holes in the unit of free-electron mass for CdS planar monolayer obtained from parabolic fitting to the CBM and VBM along different directions in the reciprocal space. The two values of effective masses of holes correspond to two degenerate states at the VBM.

Direction	m_e	m_{h1}	m_{h2}
Γ→K	0.148	0.139	--
		--	0.732
M→Γ	0.146	0.139	--
		--	0.753

For the two fold degenerate states at the VBM, the lighter holes are related to a more dispersive band than that related to heavy holes. According to the least-energy principle there will be more holes in the uppermost valance band upon light radiation, corresponding to heavy holes, thus heavy holes will be the preferred carrier transport channels.[1] Hereafter, only the effects of heavy holes (marked in red in **Table S1**) are discussed.

1 N. Umezawa, O. Shuxin, J. Ye, Phys. Rev. B 2011, 83, 035202.