Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information for

Two-Dimensional Zigzag-Shape Cd_2C Monolayer with a Desirable Bandgap and High Carrier Mobility

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Figure S1-S8: Energies of five candidate structures; FPMD snapshots of Cd_2C monolayer at 900, 1200 and 1500 K, and $Cd_2C{-}O_2/H_2O$ systems at 300 K; Compared band structure of Zn_2C and PDOS under other 2D space-groups; band structures under the ***a*** tensile and ***z*** compression strains; and fitting of CBM and VBM shift with respect to the lattice dilation or compression.

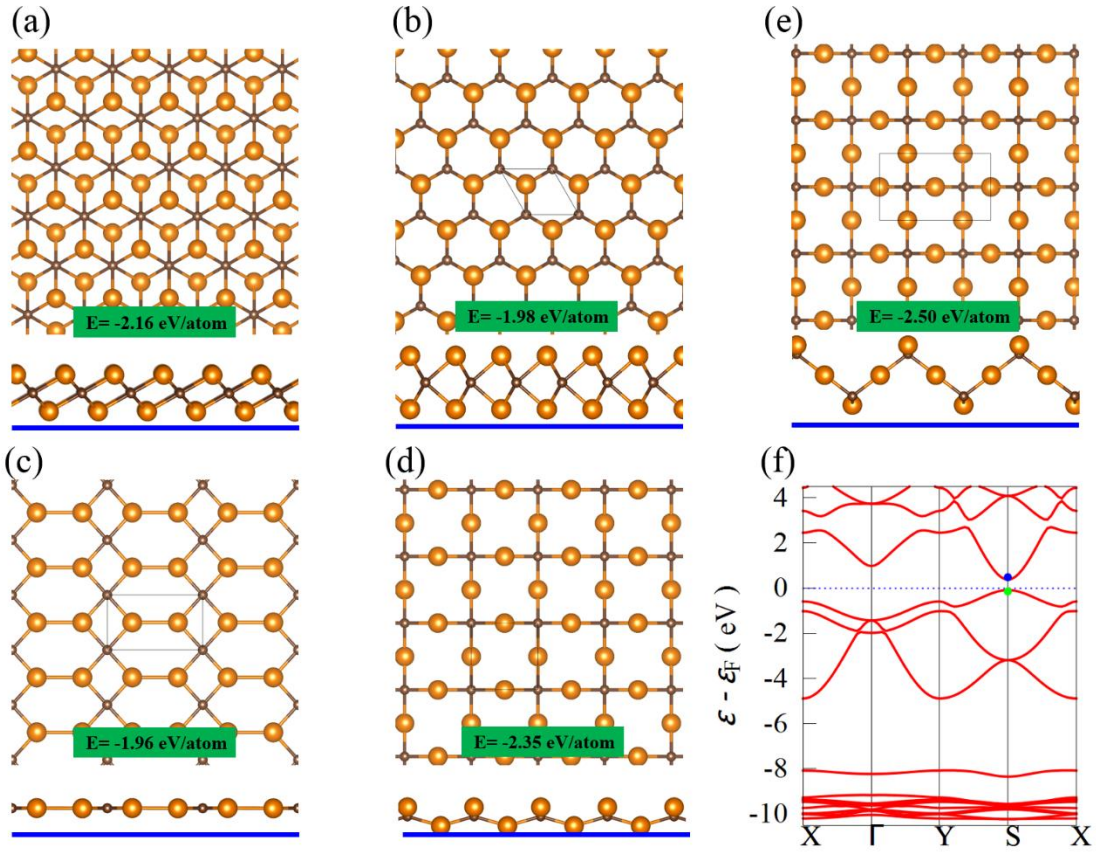

Figure S1. (a-e) Calculated energies of five candidate structures in the first approach of structural search. **e** corresponds to the structure discussed in the text. (f) HSE06 band structure of the second lowest-energy candidate **d** monolayer (presented for reference). The **d** monolayer is semiconducting with a narrow direct bandgap of ~0.68 eV (in HSE06) at S(1/2, 1/2, 0) point.

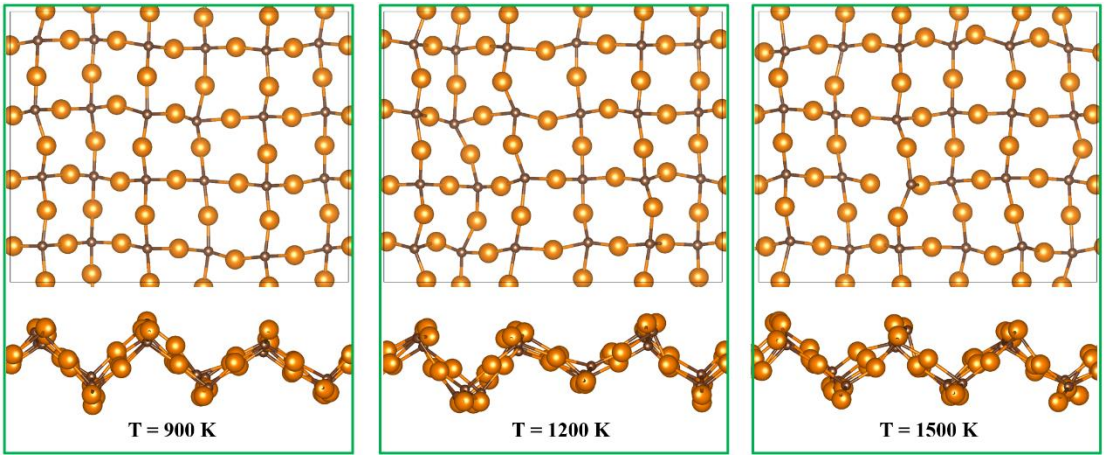

Figure S2. Structure snapshots for FPMD simulations of Cd_2C monolayer in 3×4 supercell at 900, 1200 and 1500 K.

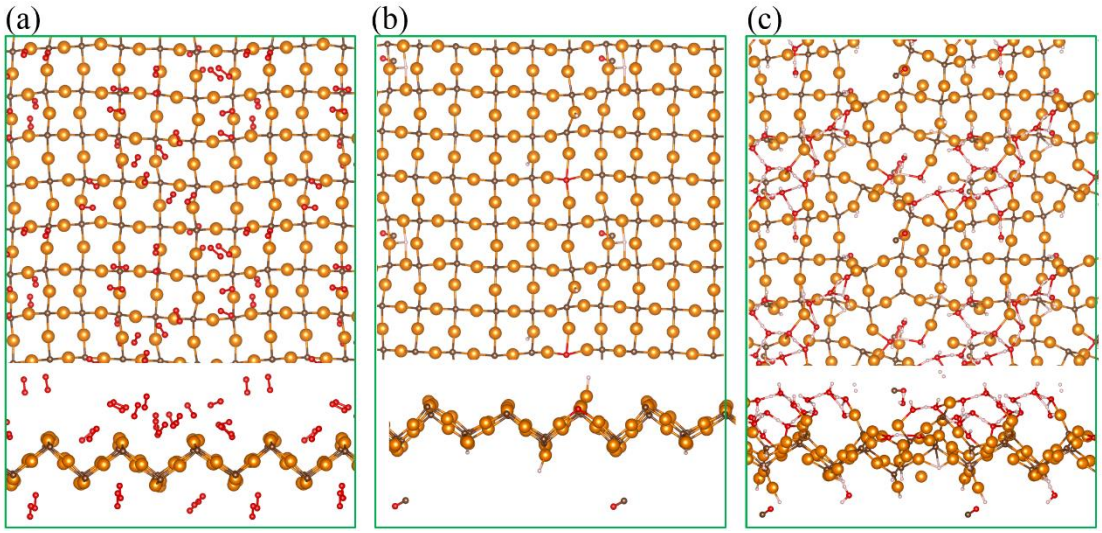

Figure S3. Structure snapshots for 300 K FPMD simulations of (a) (3×4)Cd_2C−$24O_2$, (b) (3×4)Cd_2C−$2H_2O$ and (c) (3×4)Cd_2C−$24H_2O$ systems. Note that, in (3×4)Cd_2C −$2H_2O$ with a lower density of H_2O, the sheet structural integrity can basically maintain, compared to that in (3×4)Cd_2C−$24H_2O$. Thus, in a highly dry condition with infinitesimal local damages by waters, the structure and properties of the material can be expected to remain.

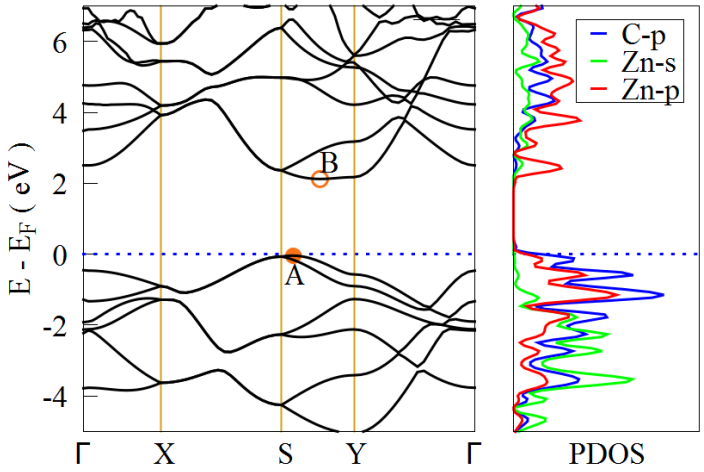

Figure S4. HSE06 band structure of Zn_2C monolayer (for comparison). The Fermi level (dot line) is set to zero. For Zn_2C monolayer, the VBM is mainly from C 2p and Zn 4p states, very similar with that the major contribution at VBM comes from C-2p and Cd-5p states in Cd_2C.

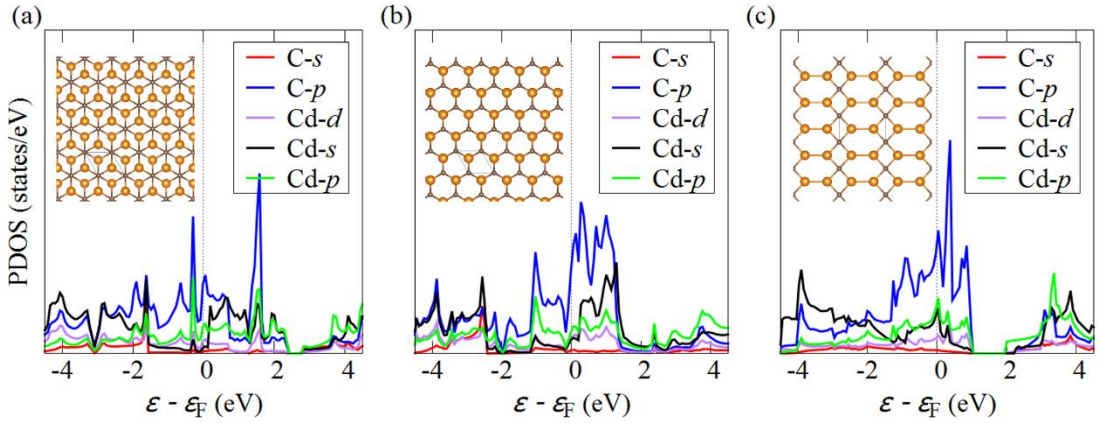

Figure S5. Projected density of states (PDOS) of Cd_2C monolayer under space-group: $P\bar{3}m1$, $P\bar{6}m2$ and *Pmmm*. The Fermi level (dot line) is set to zero.

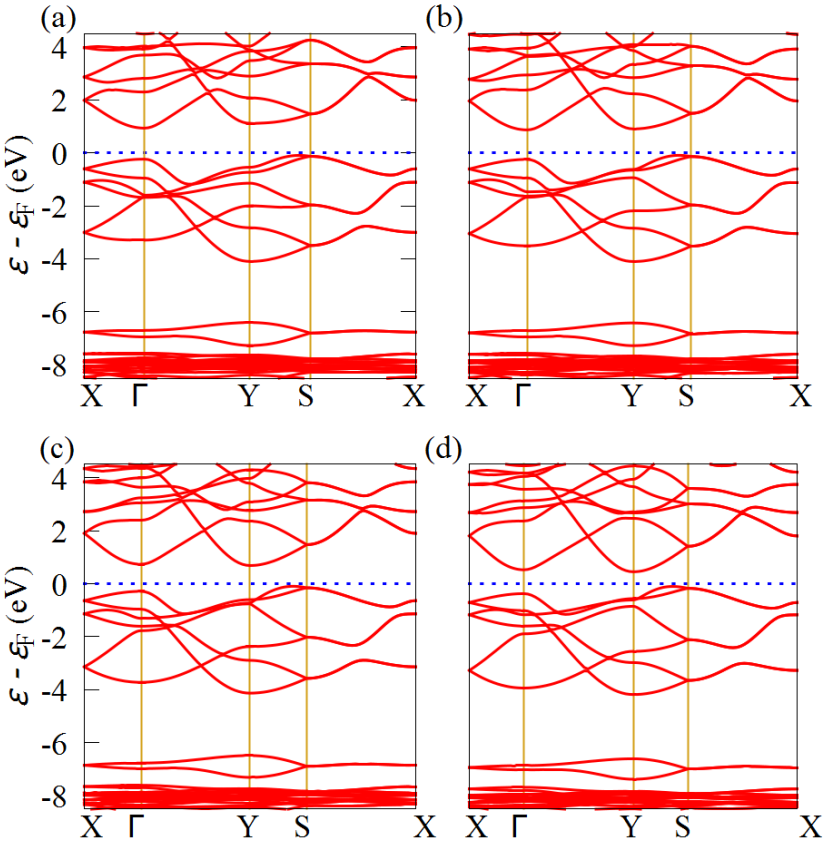

Figure S6. PBE band structures of Cd_2C monolayer under the tensile strains of (a) 5%, (b) 10%, (c) 15% and (d) 20% along ***a*** direction. The Fermi energy level is set to zero. The VBM conservers in the whole strains, while the CBM at the original Γ(0, 0, 0) point transfers to the Y(0,0,1/2) point under 15%.

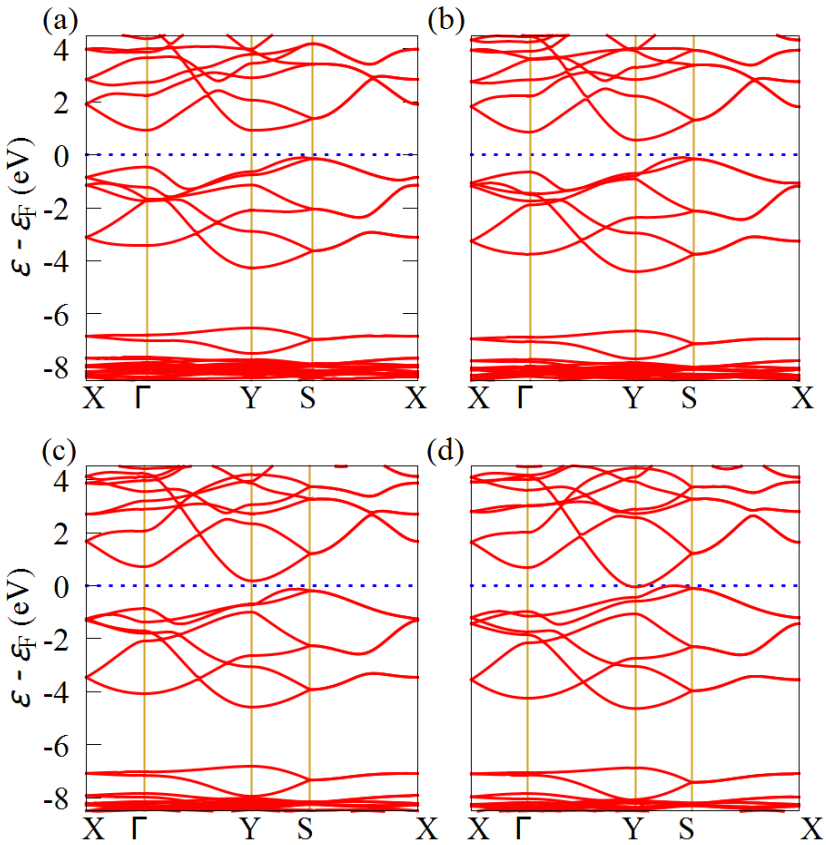

Figure S7. PBE band structures of Cd_2C monolayer under the compression strains of (a) 10%, (b) 20%, (c) 30% and (d) 40% along ***z*** direction. The Fermi energy level is set to zero. The VBM conservers in the whole strains, while the CBM at the original Γ(0, 0, 0) point transfers to the Y(0,0,1/2) point under 10%.

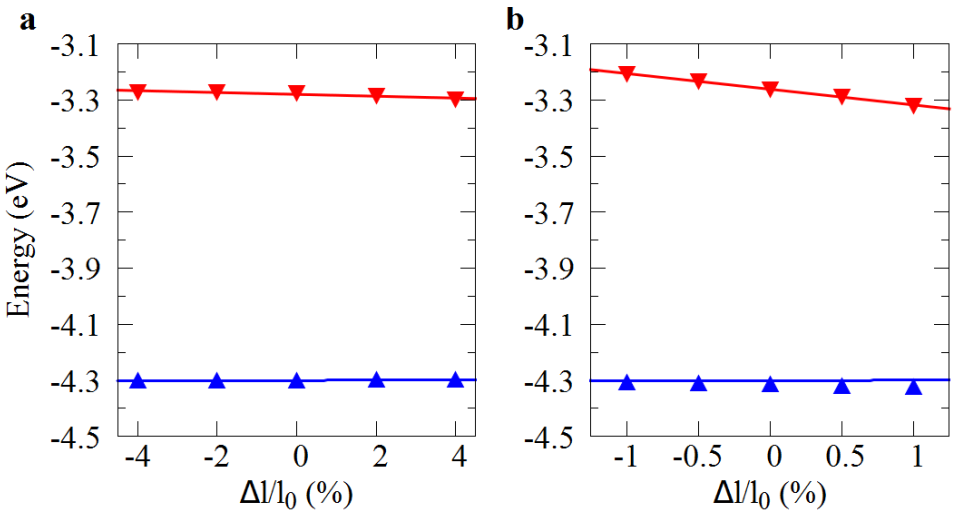

Figure S8. Linear fitting of the CBM and VBM shift (Δv) with respect to the lattice dilation or compression ($\Delta l/l_0$) along (a) ***a*** direction and (b) ***b*** direction.