Supporting Information

Promising Photocatalysts for Water Splitting in BeN_2 and MgN_2 Monolayers

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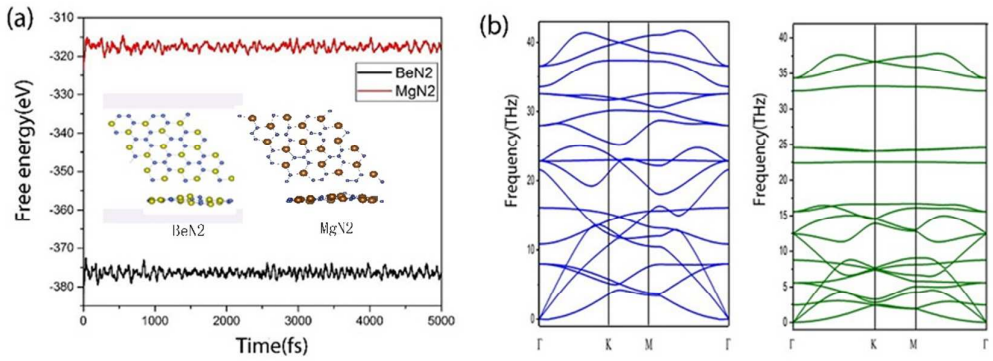

Fig. S1 (a) Variation of free energy during AIMD simulation at 800 K for BeN_2 and MgN_2 monolayers. (b) Phonon dispersion curves of BeN_2 (left) and MgN_2 (right) monolayers.

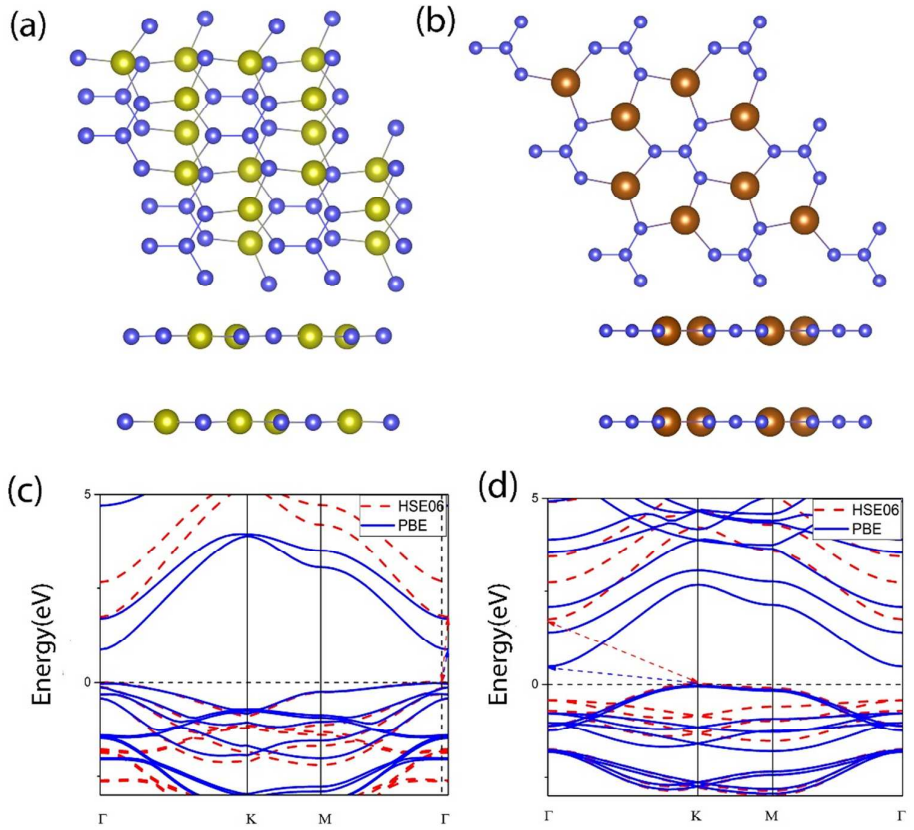

Fig. S2 (a) (b) the most stable configure after optimization for BeN_2 and MgN_2 double layers. (c) (d) the band structure of BeN_2 and MgN_2 double layers.

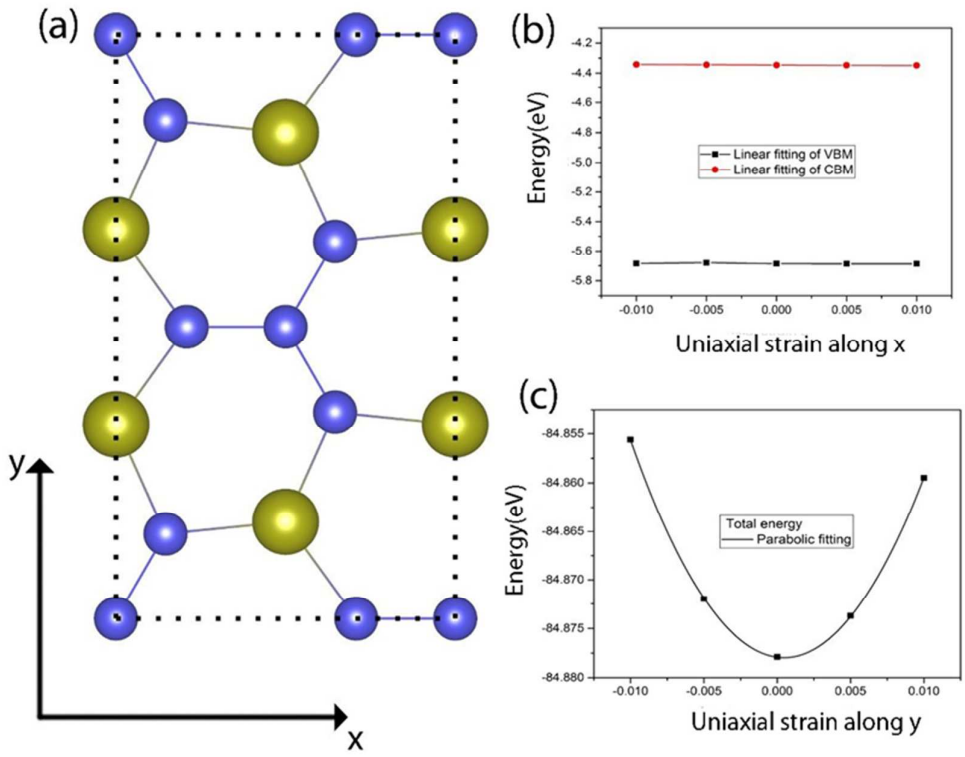

Fig. S3 (a) Rectangle unit cell of BeN_2 and MgN_2 monolayers. (b) CBM and VBM of BeN_2 monolayers along x direction as a function of deformation proportion. The solid line is a quadratic fitting to the data. (c) The energy of BeN_2 monolayers as a function of the uniaxial strain along x directions.