Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary information

A first-principles and machine-learning investigation on the electronic, photocatalytic, mechanical and heat conduction properties of nanoporous C_5N monolayer

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Atomic lattices in VASP POSCAR format.

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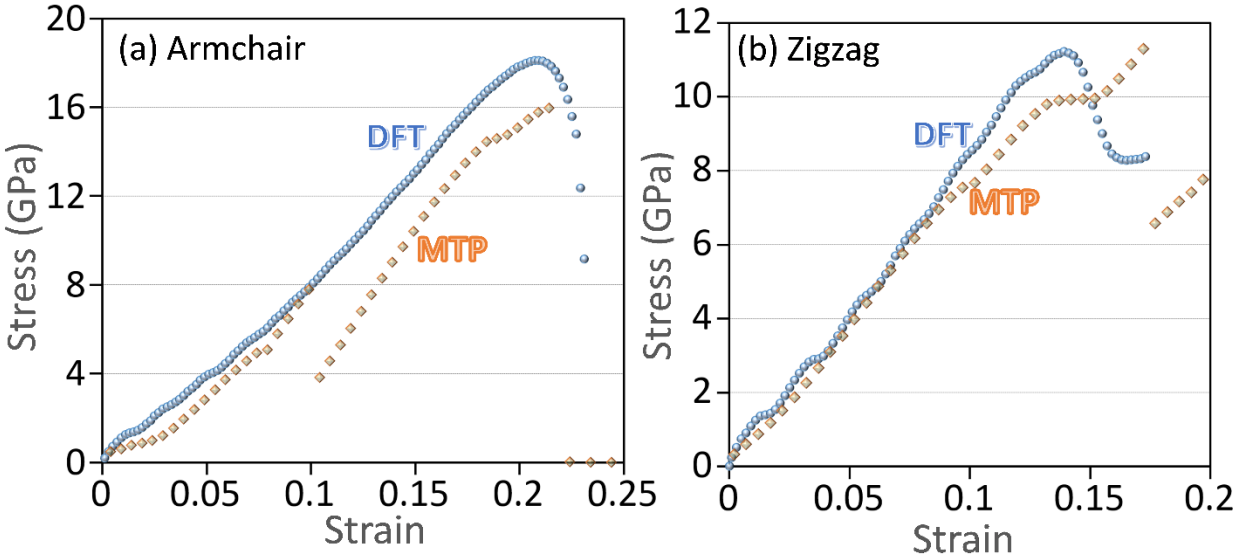

Fig. S1, Uniaxial stress-strain relations of the C_5N monolayer elongated along the (a) armchair and (b) zigzag directions by DFT and MTP-based CMD without taking into account the van der Waals (vdW) dispersion correction in the development of the MTP.

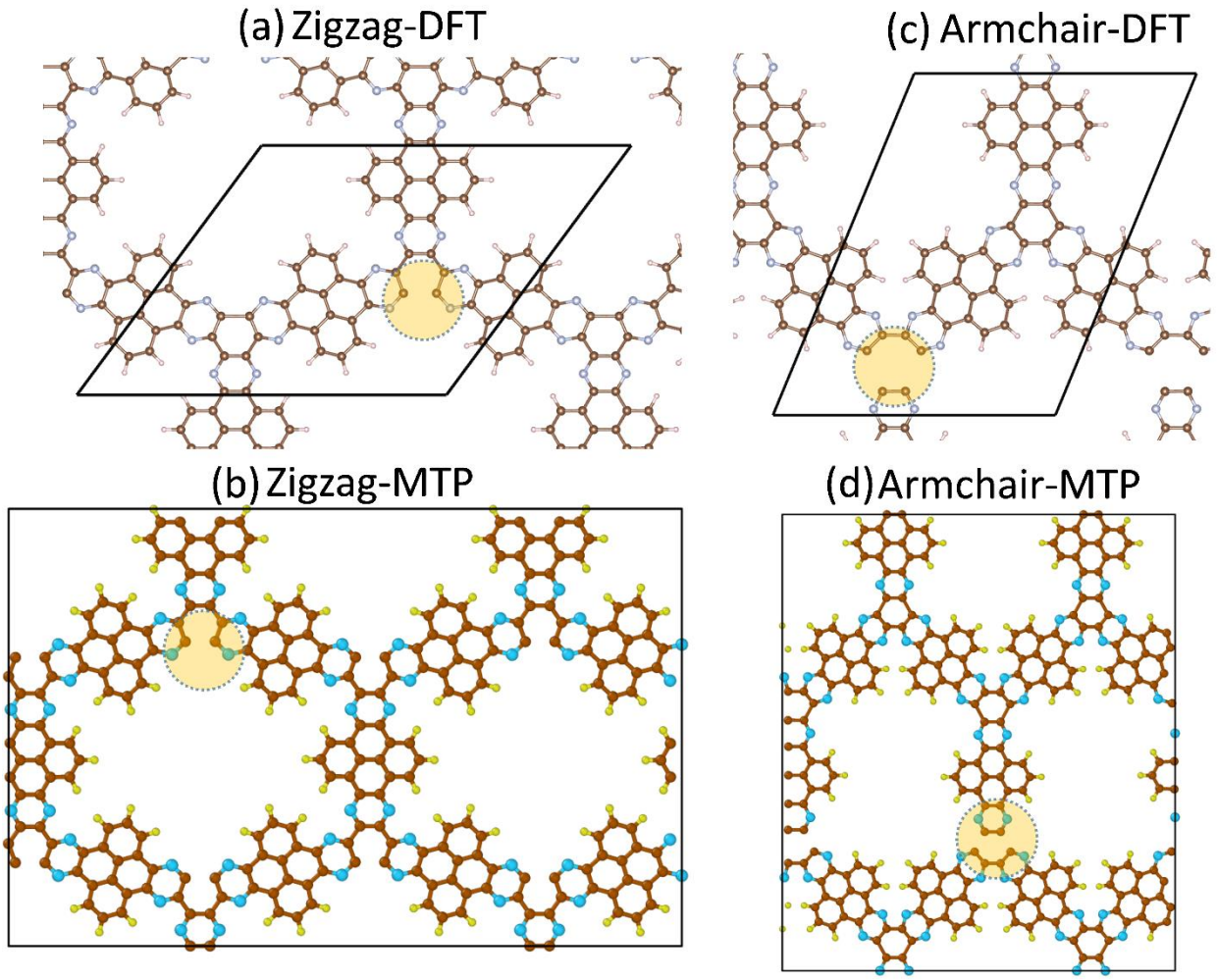

Fig. S2, Failure mechanism of the C_5N monolayer predicted by DFT and MTP-based CMD models without taking into account the vdW dispersion correction in the development of the MTP. The circles highlight the region that the bond breakages occur.