
Article:
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Supplementary Information for

Computational design of graphitic carbon nitride photocatalysts for water splitting

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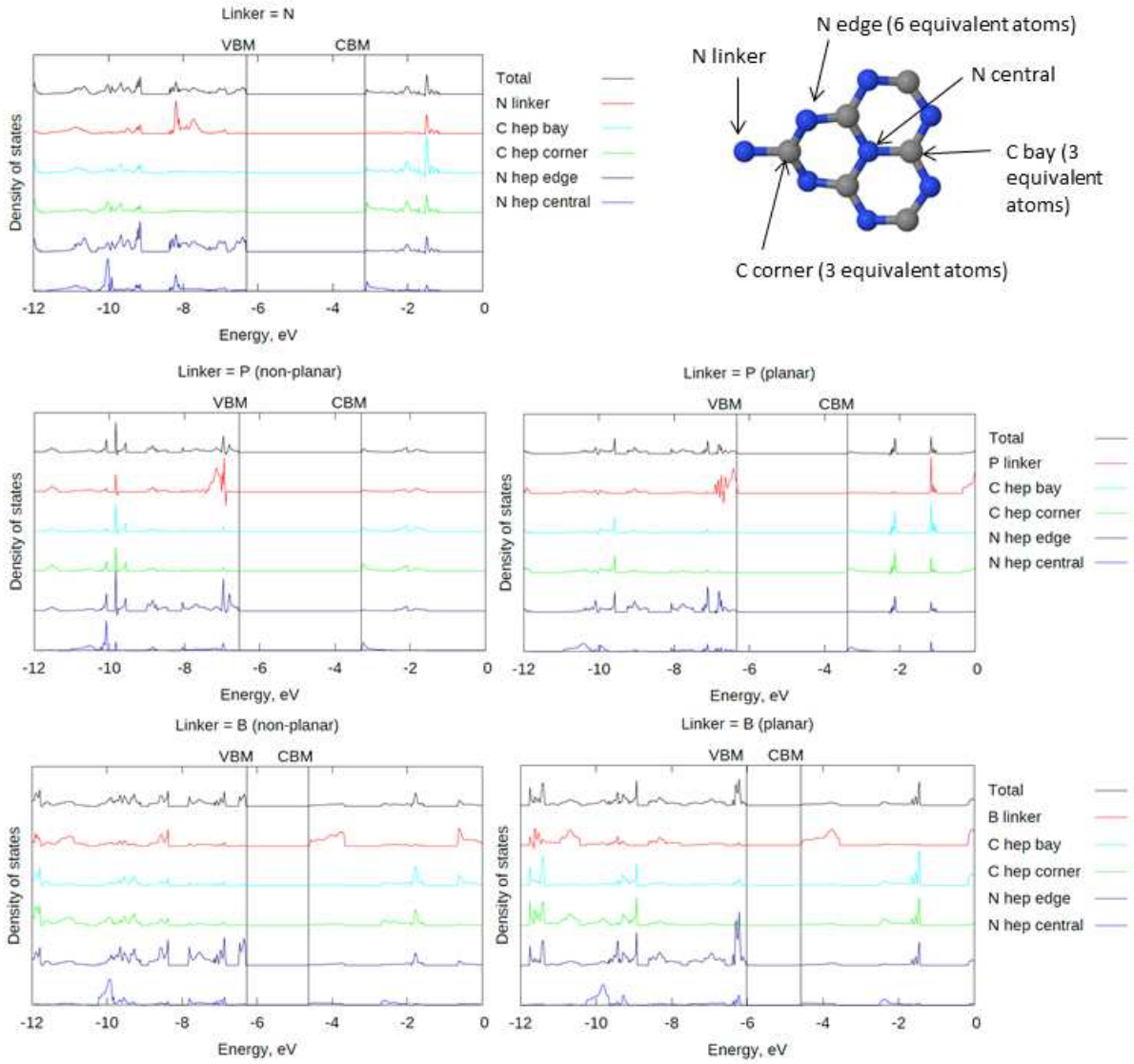

Figure S1. Projected densities of states for N-, P- and B-linked graphitic carbon nitride structures. Atom types (N central, edge and linker, C bay and corner) are indicated. The zero energy is the energy of electron in vacuum.

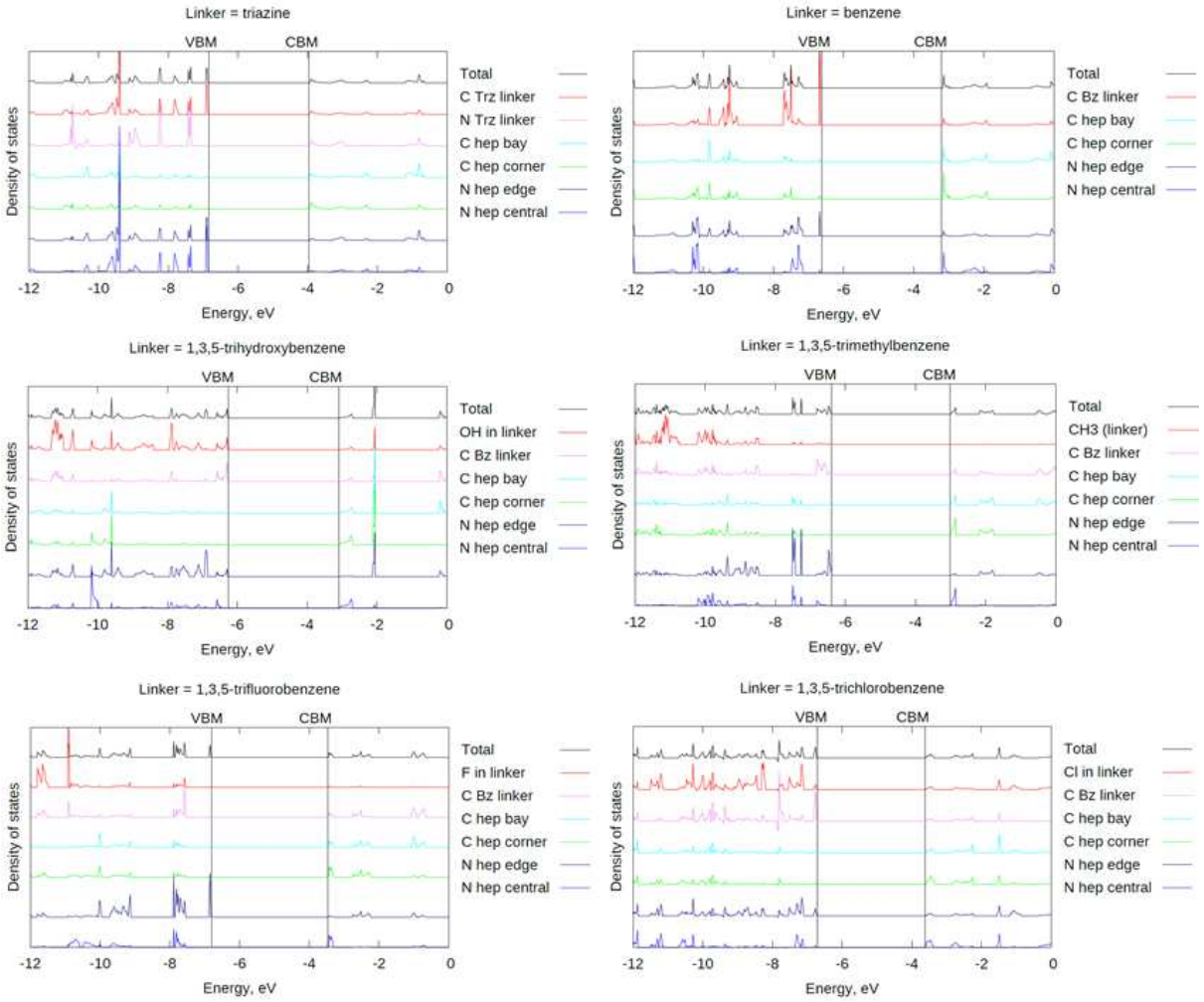

Figure S2. Projected densities of states for triazine-, benzene- and substituted benzene-linked graphitic carbon nitride structures. The zero energy is the energy of electron in vacuum.

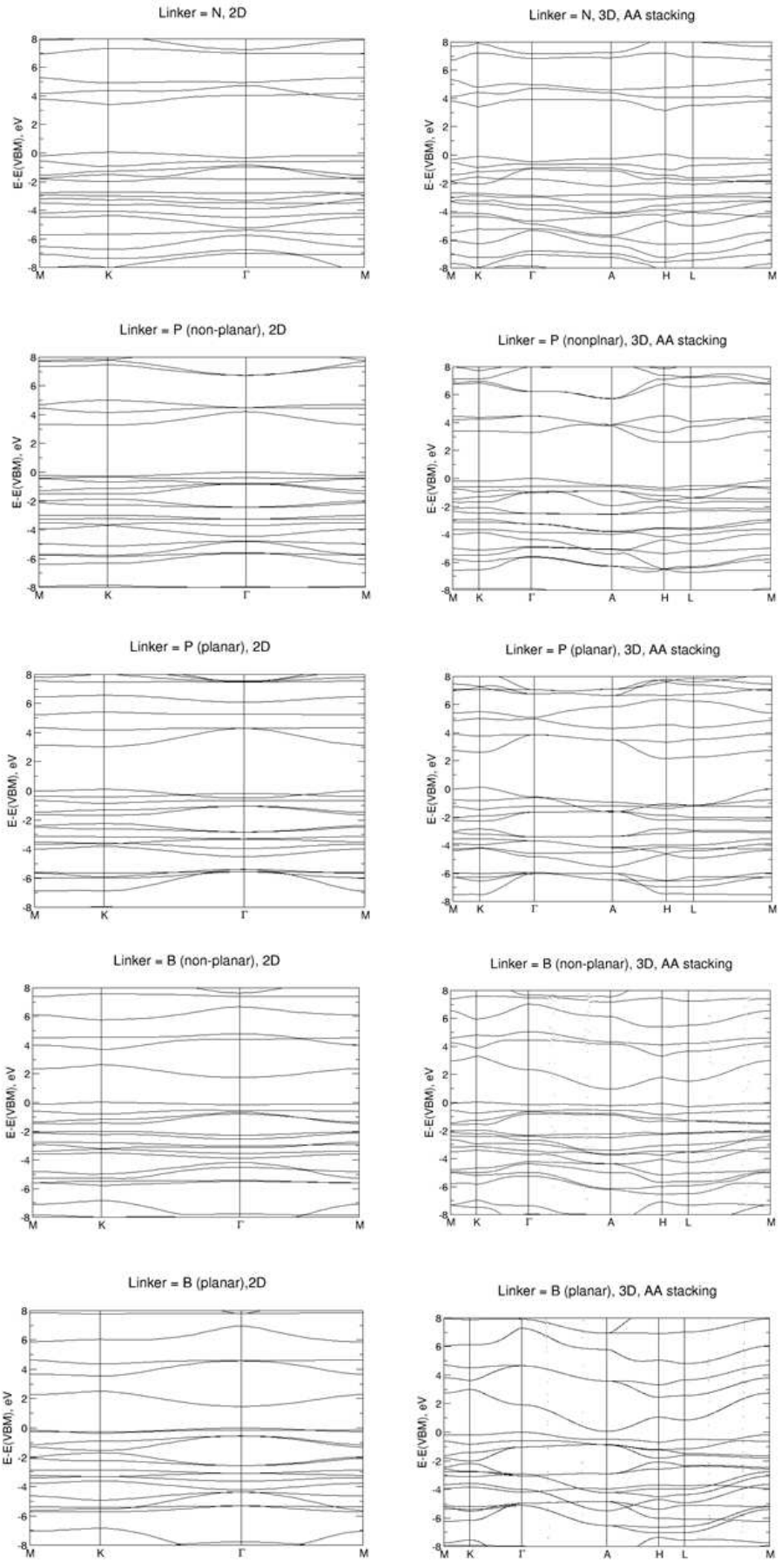

Figure S3. Band structure plots for N-, P- and B-linked graphitic carbon nitrides (2D and 3D AA-stacked structures). The zero energy is at the top of the valence band.

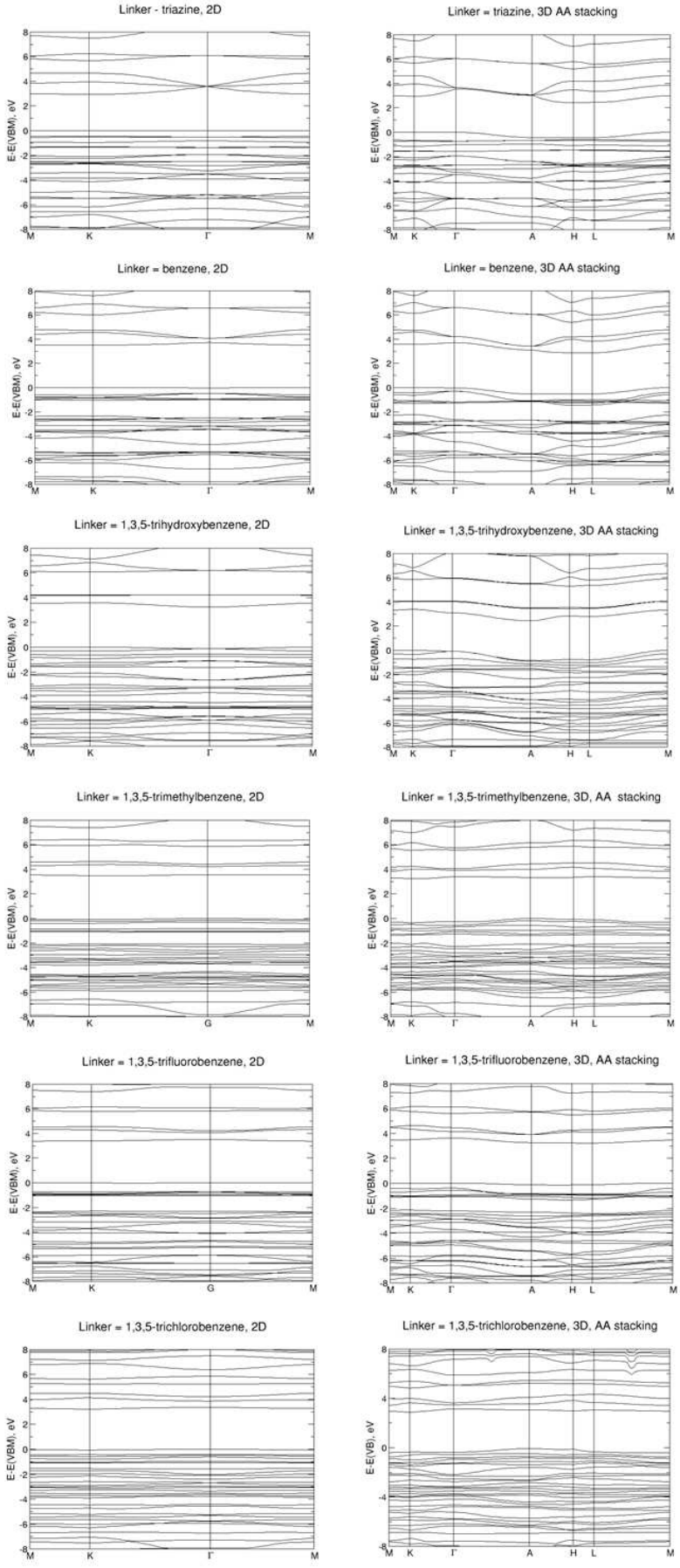

Figure S4. Band structure plots for triazine-, benzene- and substituted benzene-linked graphitic carbon nitrides (2D and 3D AA-stacked structures). The zero energy is at the top of the valence band.