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

Photocatalytic Splitting of Water on *s*-triazine based Graphitic Carbon Nitride: An *ab initio* Investigation

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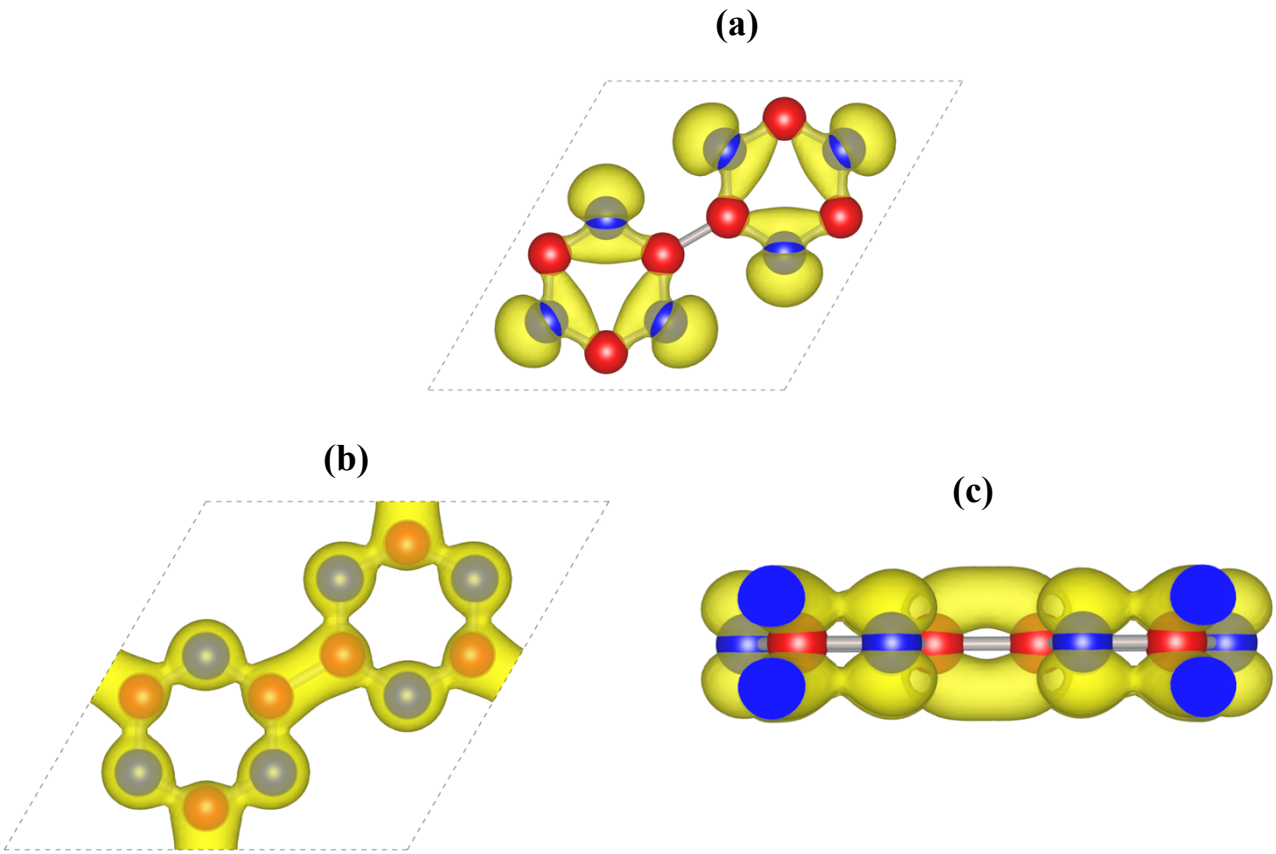

Figure S1. Band decomposed change density iso-surfaces of (a) valence band maxima and conduction band minima in (b) top-view and (c) side view

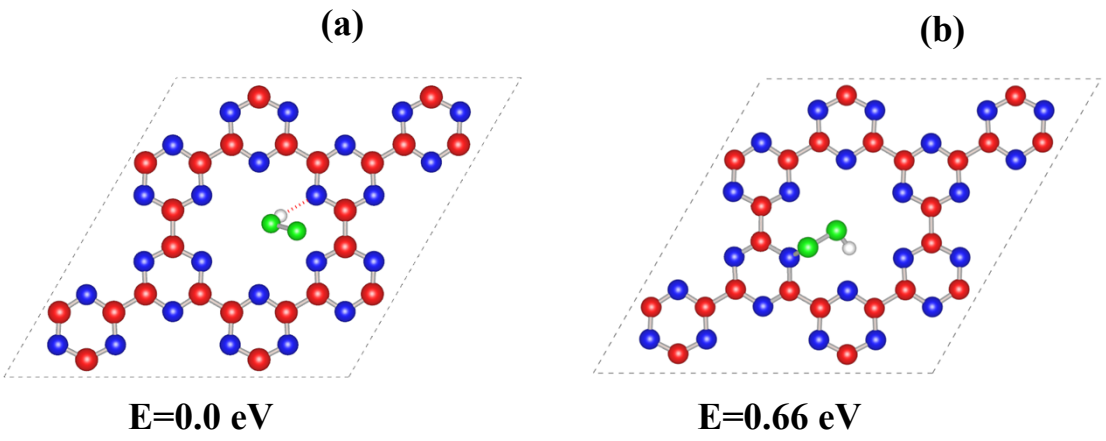

Figure S2. Optimized conformers of g-CN-OOH (a) hydrogen bonded with out any N-O bond and (b) chemisorbed on g-CN through N-O bond formation along with energy differences

Minimum Energy Path calculations:

To calculate the minimum energy path (MEP) we considered eight images (including the initial and final geometries) along the reaction path. Climbing image nudge elastic band (CI-NEB) method has been used to get the transition state. Geometries of all the images with energies were given below in Figure S2. Quantum Espresso program has been used to do the CI-NEB calculations with plane wave energy cut-off of 40 Ry. 3x3x1 automatically generated k-mesh has been used for sampling the Brillouin zone.

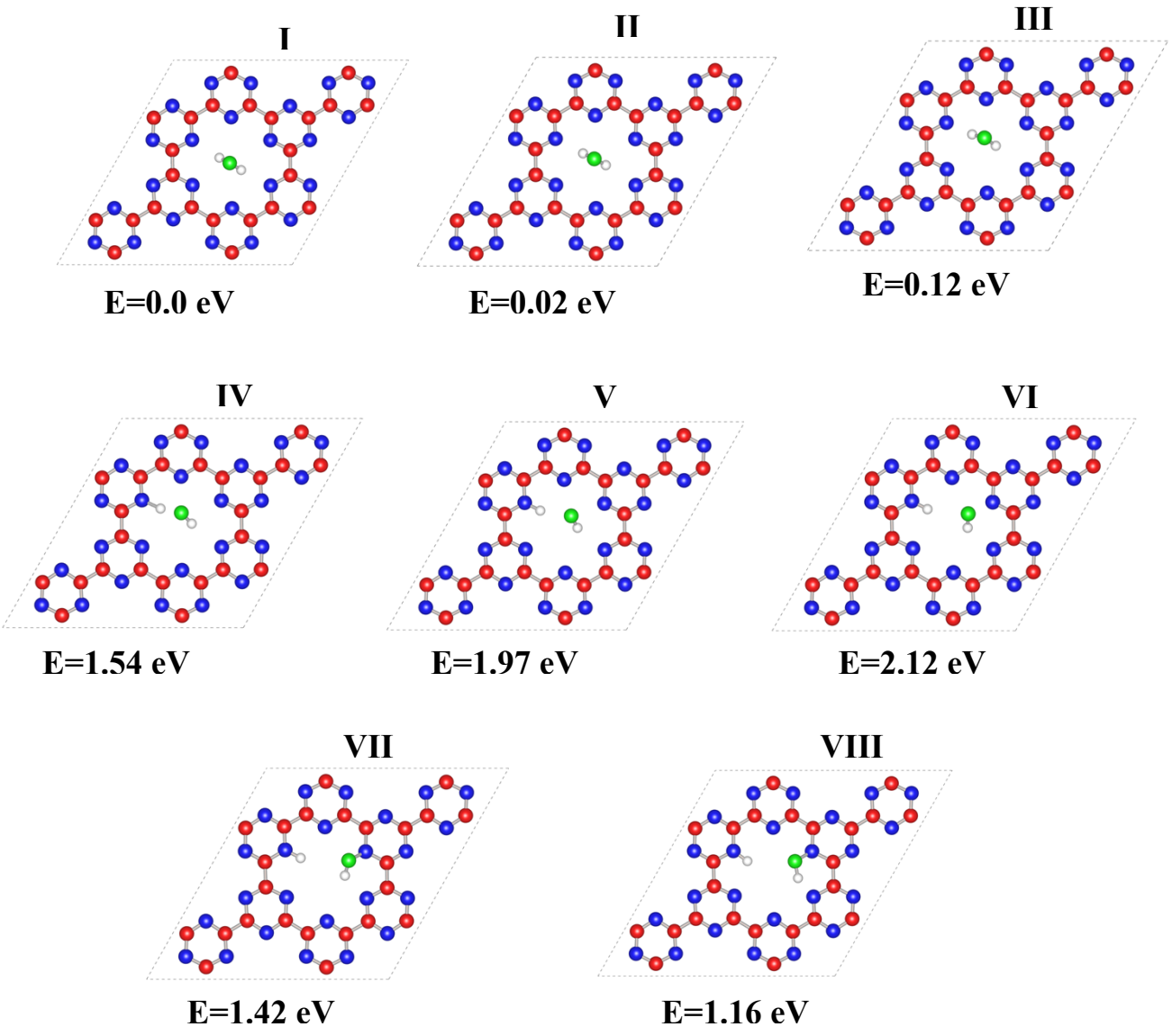

Figure S2. Geometries of the images along with their energies with respect to the images I in eV.