Atomic chemisorption on graphene with Stone–Thrower–Wales defects

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Using first-principles calculations, we investigate the chemisorption of H, N, and P atoms on a graphene substrate with or without Stone–Thrower–Wales (STW) defects. Energetically, all three atoms are preferred to adsorb onto the defect sites by an energy difference of 0.683–2.143 eV. In both the intrinsic and defected graphene, H atom adsorbs on top of a C atom, while N and P atoms adsorb at the bridge site between two C atoms with the N atom breaking the underneath C–C bond in the STW defect. Changes of atomic, electronic and magnetic structures associated with the atomic chemisorption on STW defects in graphene are discussed.

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