Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Origin of the half-metallic properties of graphitic carbon nitride in bulk and confined form

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1. Frontier molecular orbitals of the isolated sym-triazine and benzene molecules

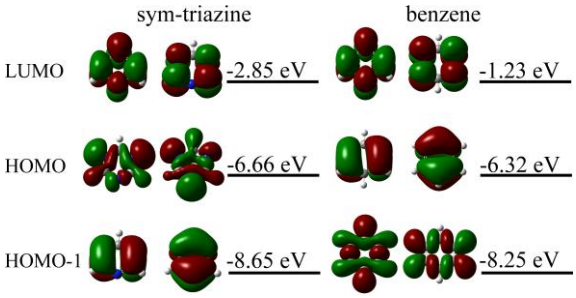

Figure S1 Comparison of the frontier molecular orbitals of the isolated sym-triazine and benzene molecules calculated at the PBEPBE/6-311+G(d,p)

2. Optimized atomic structures and the corresponding spin-resolved band structures of zigzag g-C_4N_3 nanoribbons passivated with methyl groups

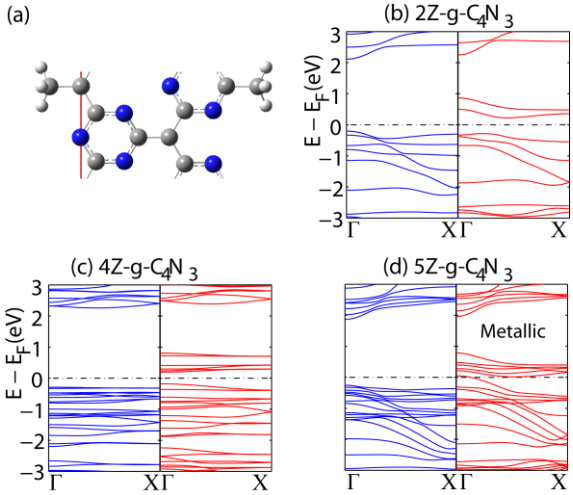

Figure S2 (a) The optimized atomic structure of the 2Z-g-C_4N_3 nanoribbon passivated with methyl groups, and the corresponding spin-polarized band structures of the 2Z-g-C_4N_3 (b), 4Z-g-C_4N_3 (c) and 5Z-g-C_4N_3 (d) nanoribbons

3. Optimized atomic structures and the corresponding spin-resolved band structures of armchair g-C_4N_3 nanoribbons passivated with methyl groups

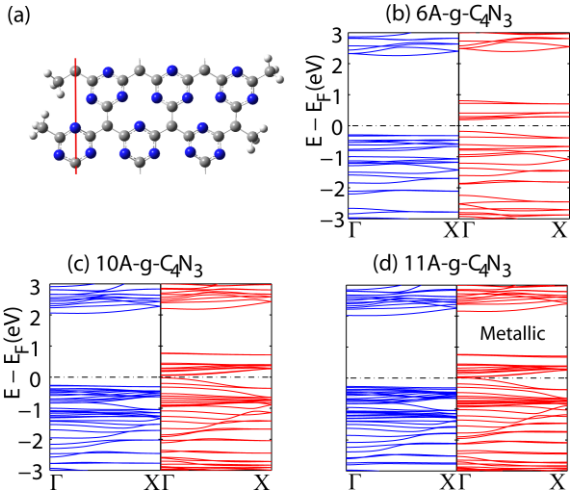

Figure S3 (a) The optimized atomic structure of the 6A-g-C_4N_3 nanoribbon passivated with methyl groups, and the corresponding spin-polarized band structures of the 6A-g-C_4N_3 (b), 10A-g-C_4N_3 (c) and 11A-g-C_4N_3 (d) nanoribbons