Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Insights into enhanced visible-light photocatalytic activity of C_{60} modified g-C_3N_4 van der Waals heterostrutures: the role of unsaturated nitrogen

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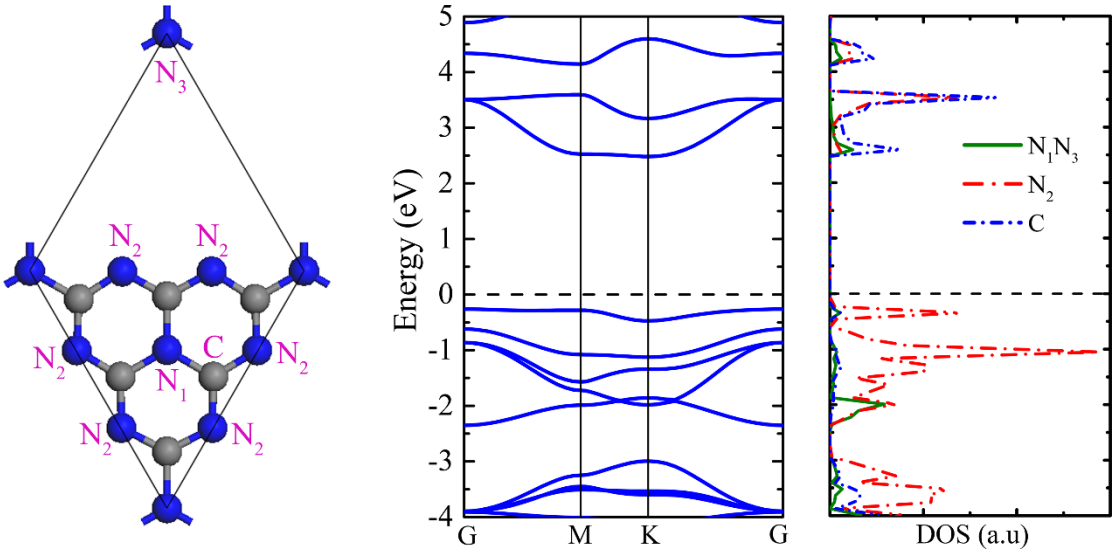

Figure S1 Optimized geometric structure (left), band gap (middle), and PDOS (right) of the primitive cell for g-C_3N_4 monolayer. The Fermi level is set to zero.

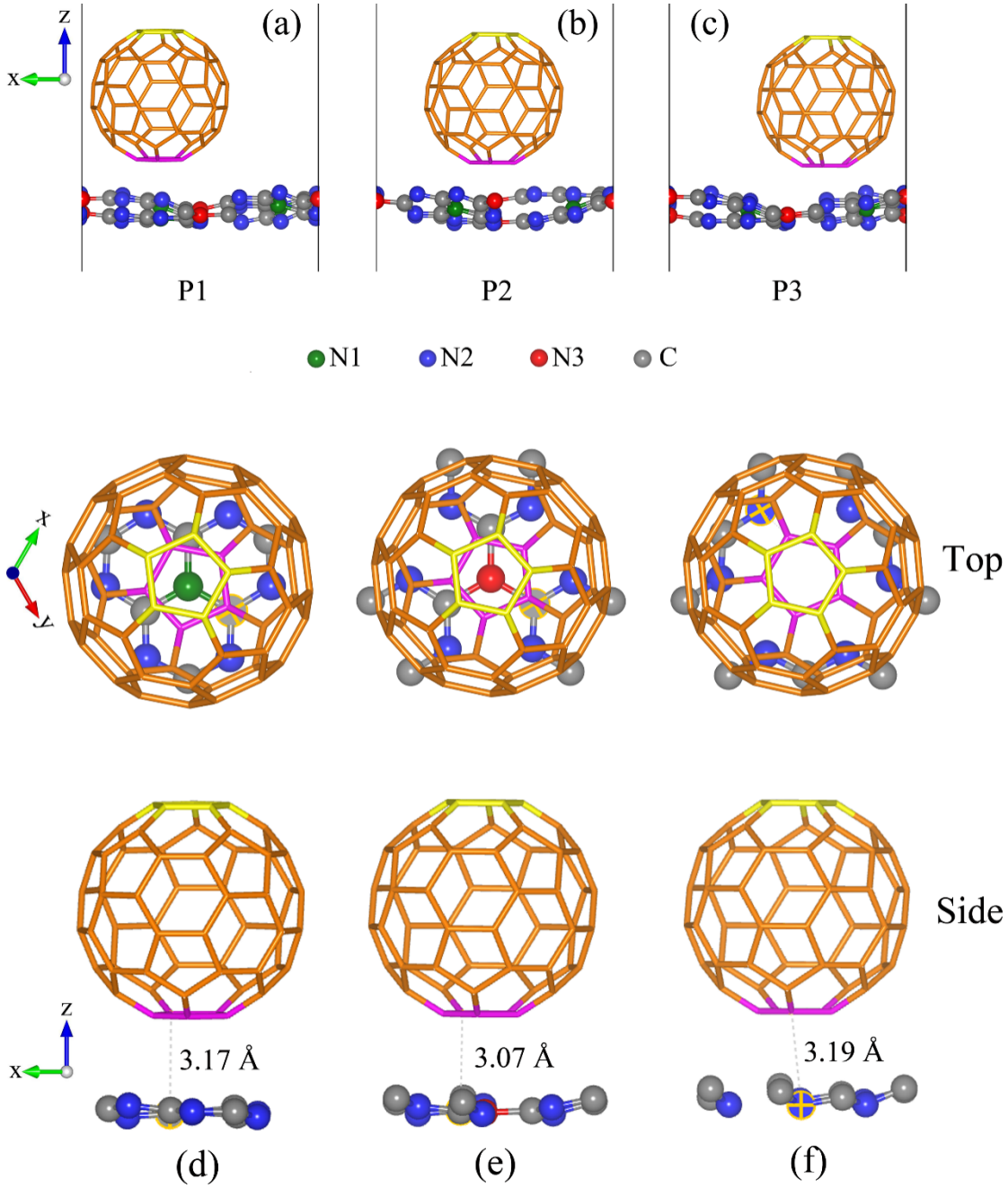

Figure S2 Side view of (a) P_1, (b) P_2, and (c) P_3. Top and side views of the interfacial regions for (d) P_1, (e) P_2, and (f) P_3. The N_1, N_2, N_3, and C atoms are denoted by green, blue, red, and gray spheres, respectively. The shortest atomic spacing between the two different constituents (d_2) is labeled by dotted line.

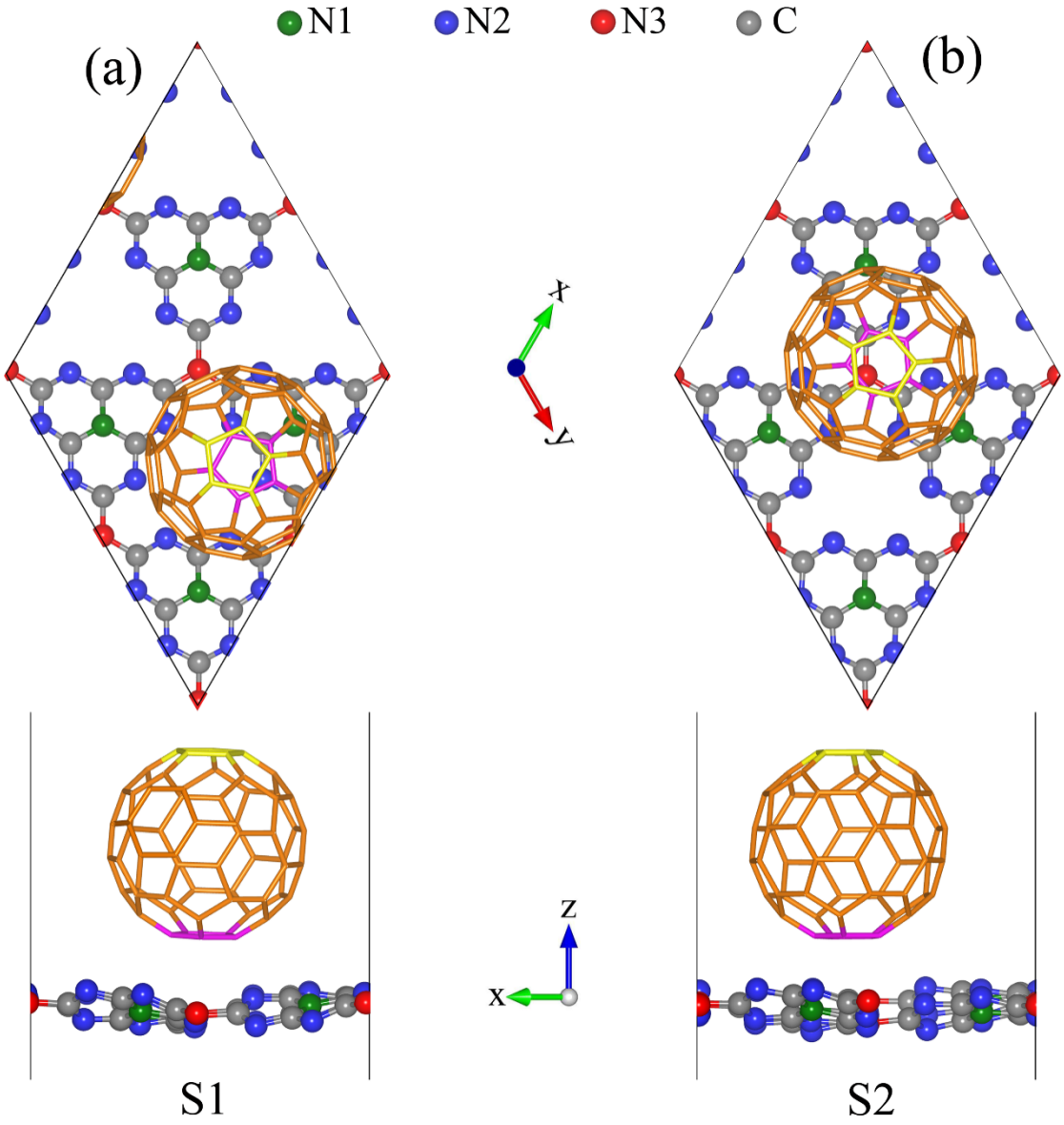

Figure S3 Top and side views of two asymmetric C_{60}/g-C_3N_4 nanocomposites, labeled as (a) S_1 and (b) S_2, respectively. The N_1, N_2, N_3, and C atoms are denoted by green, blue, red, and gray spheres, respectively.

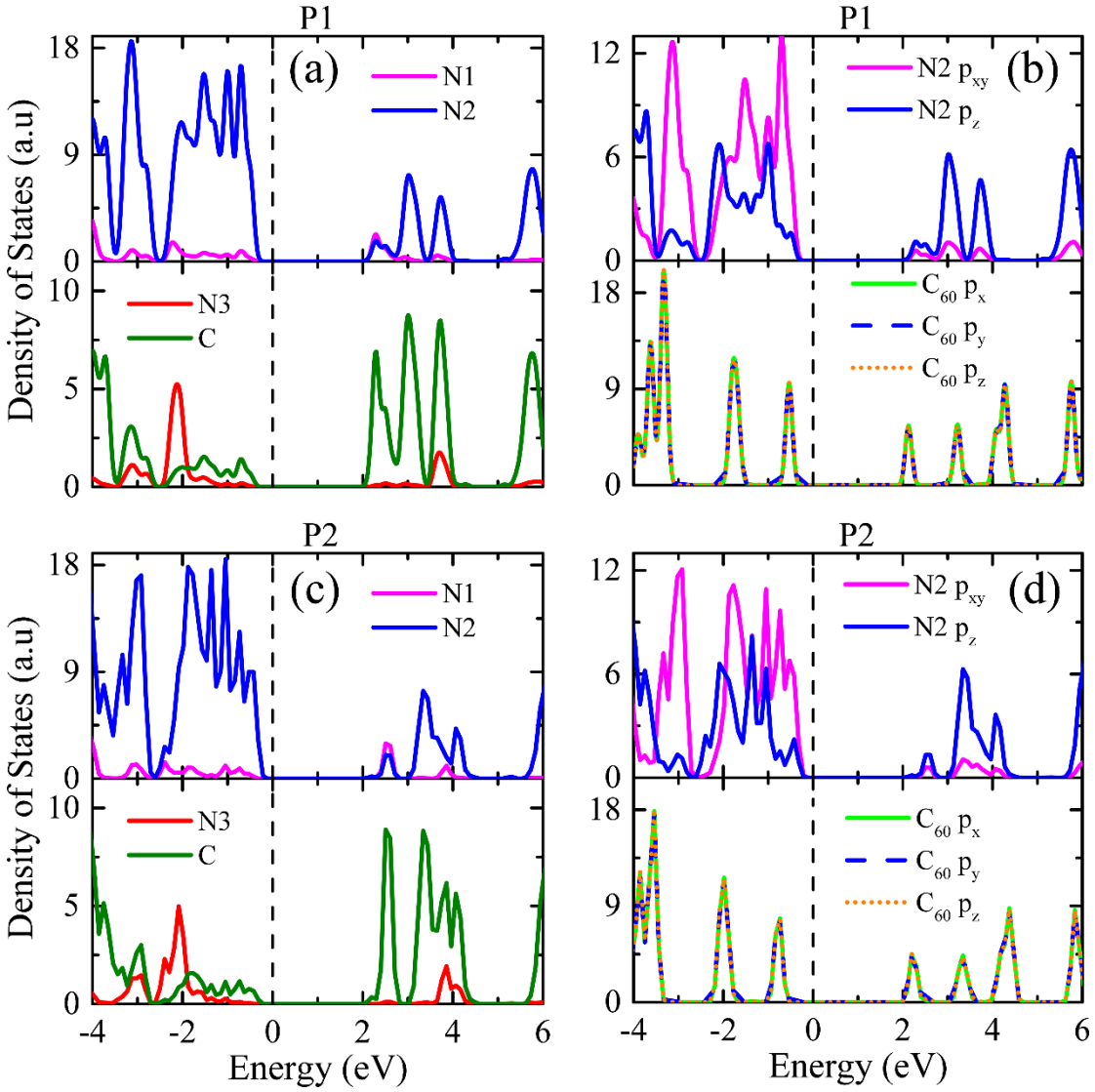

Figure S4 (a) PDOS and (b) Orbital-decomposed DOS of P_1, (c) PDOS and (d) Orbital-decomposed DOS of P_2. The Fermi level is set to zero.

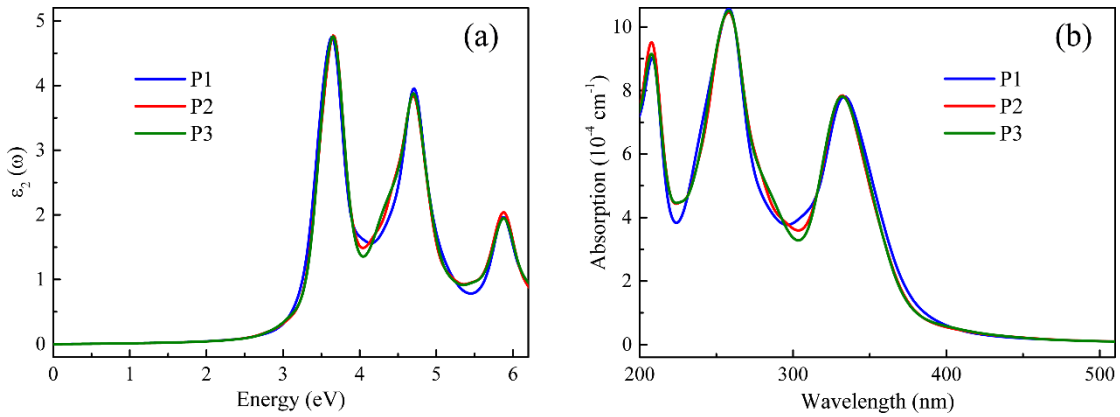

Figure S5 Calculated (a) imaginary part of the dielectric function and (b) absorption spectra of P_1, P_2, and P_3 for the polarization vector perpendicular to the surface.

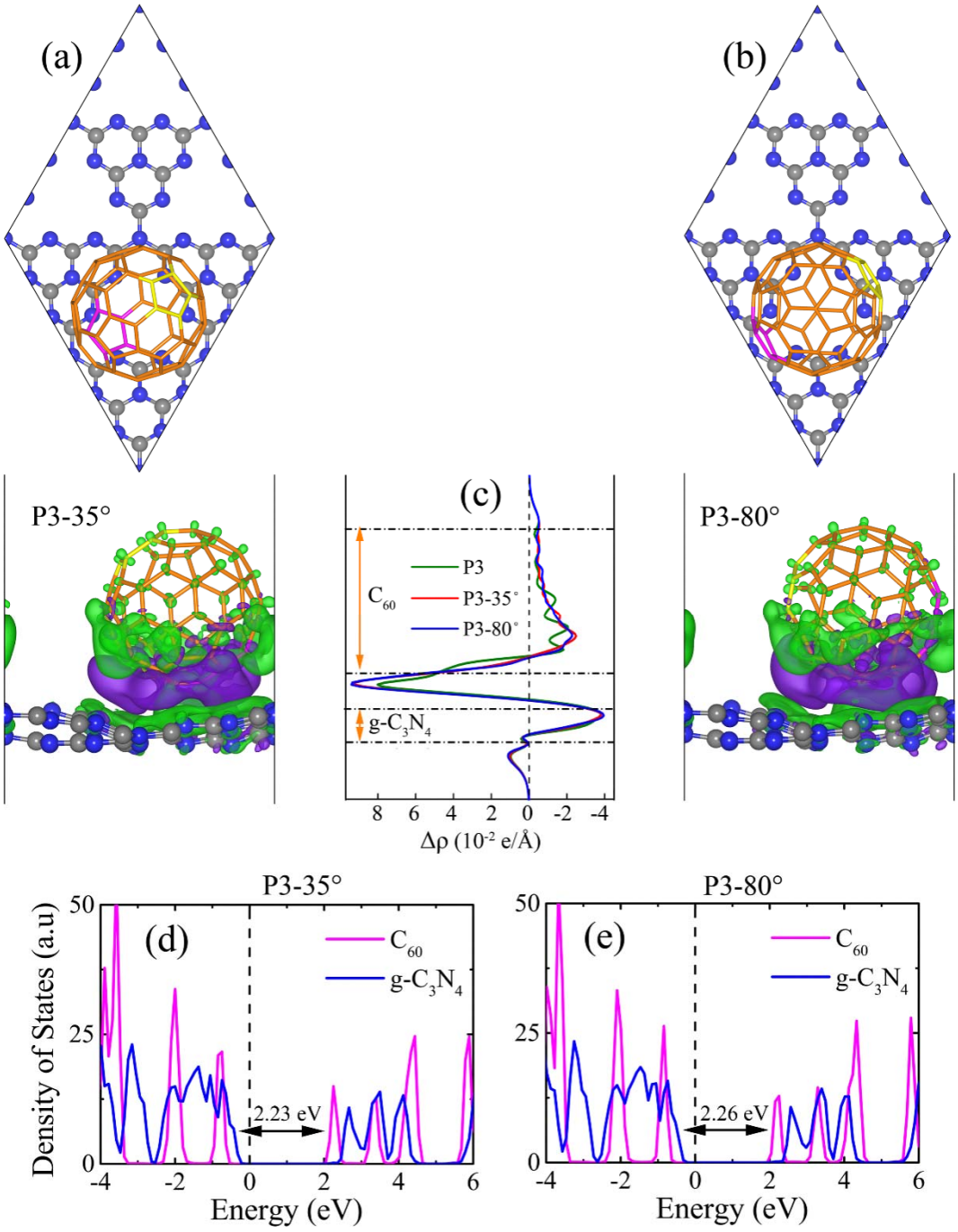

Figure S6 Top view and 3D charge density difference of (a) P_3-35° and (b) P_3-80° with an isovaule of 0.001 e/Å^3. Purple and cyan isosurfaces denote charge accumulation and depletion in the space, respectively. (c) Profile of planar averaged self-consistent electrostatic potential for P_3, P_3-35°, P_3-80°, as a function of position in the z-direction. PDOS of P_3-35° and P_3-80°, with the band gaps of 2.23 eV and 2.26 eV, respectively. The Fermi level is set to zero.