Field-screening Ability of Pentagonal sp2 Carbon Networks

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The electronic structure of nanoscale materials affects their electrostatic properties. For instance, the capacitance of carbon nanotubes is highly sensitive to their density of states (DOS). Two-dimensional (2D) carbon networks often possess flat dispersion bands [1,2], leading to a large DOS at the Fermi level. These 2D carbon networks are expected to exhibit a remarkable response to external fields. Thus, in this work, we aim to investigate the field-screening ability of 2D carbon networks with a large DOS at or near the Fermi level under an electric field using density functional theory with the effective screening medium method.

We focus on three representative 2D carbon networks comprising pentagonal rings of sp2 carbon atoms, possessing a large DOS at or near the Fermi level [Fig. 1]. By applying the electric field, the relative permittivity of a fused pentagon network, a symmetrically hydrogenated fused pentagon network, and an asymmetrically hydrogenated fused pentagon network is 2.14, 2.00, and 2.10, respectively, which are similar to the graphene value of 2.19. This permittivity is due to the competition between the charge density and polarized carrier attributed to the large DOS at the Fermi level.

References

[1] M. Maruyama, S. Okada, Appl. Phys. Express 6, 095101 (2013).
[2] T. Mizoguchi et al. Phys. Rev. B 112, 085421 (2025).

Figure

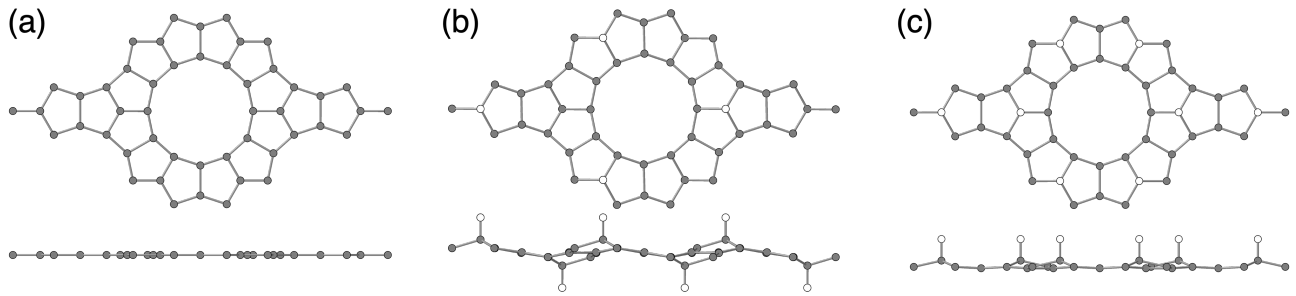

Figure 1: Geometries of (a) fused pentagon network, (b) symmetrically hydrogenated fused pentagon network, and (c) asymmetrically hydrogenated fused pentagon network.