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Electronic Transport in C-57 and Its Hydrogenated Derivative

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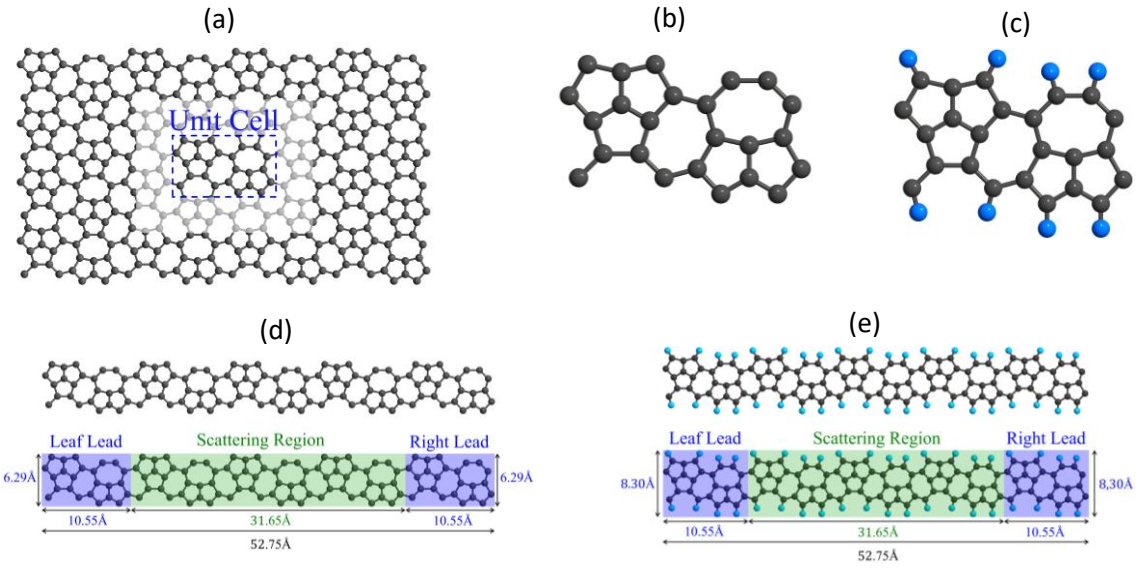
Abstract

Nanoscience and nanotechnology have revolutionized materials research. This study investigates the electronic transport properties of carbon C-57 and its hydrogenated derivative using Density Functional Theory (DFT) combined with Non-Equilibrium Green's Function (NEGF) methods. Our findings reveal distinct behaviors: C-57 exhibits a decrease in current with increasing voltage due to limited available electronic states for conduction. In contrast, hydrogenated C-57 demonstrates a near-constant current with an interesting increase in the 0.42-0.50 V range. This is attributed to increased conductance resulting from a greater density of states near the Fermi level and reduced potential barriers. These results suggest that C-57 and hydrogenated C-57 possess unique electronic properties with potential applications in molecular electronics and nanoscience.



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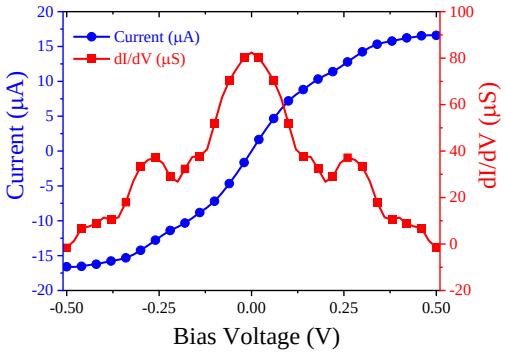

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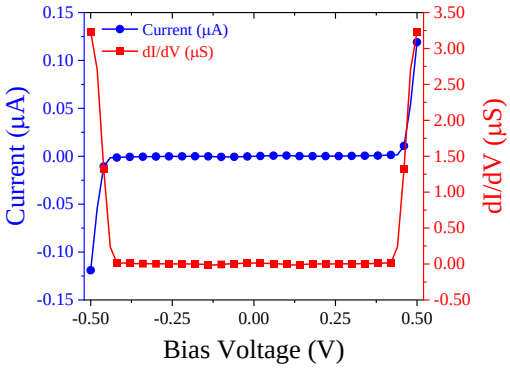

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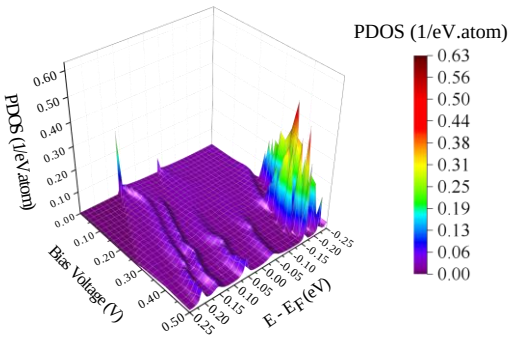

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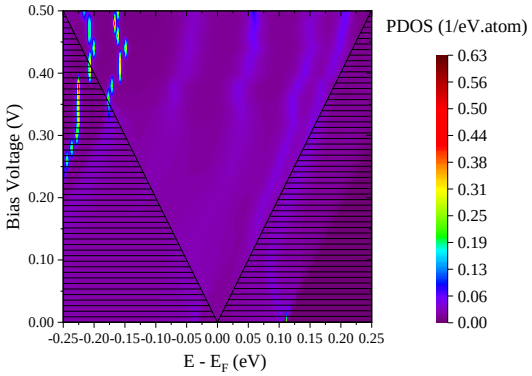

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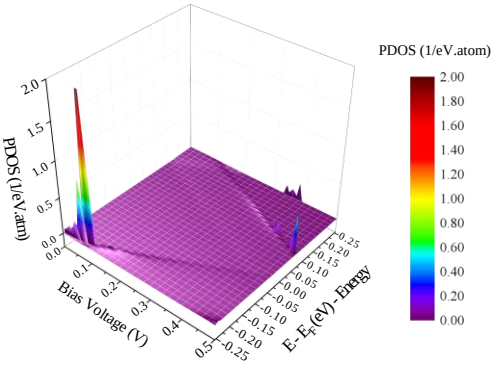

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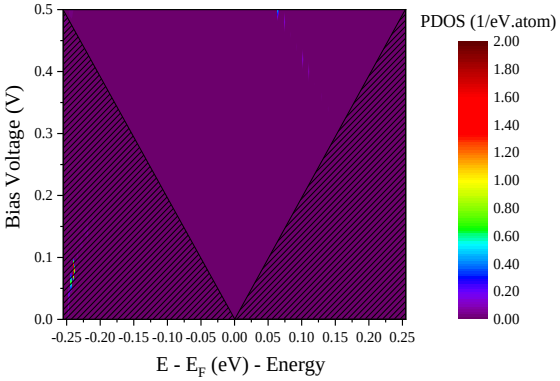

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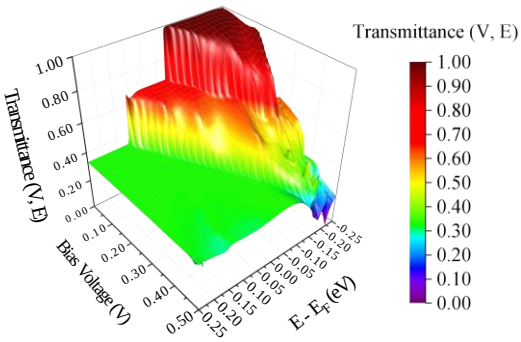

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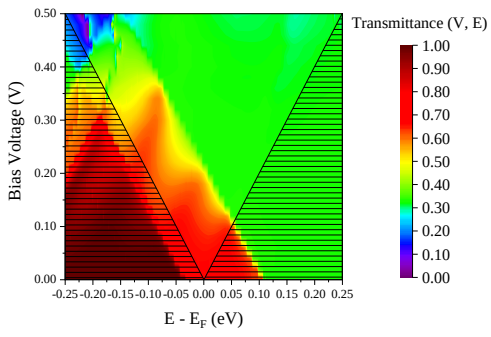

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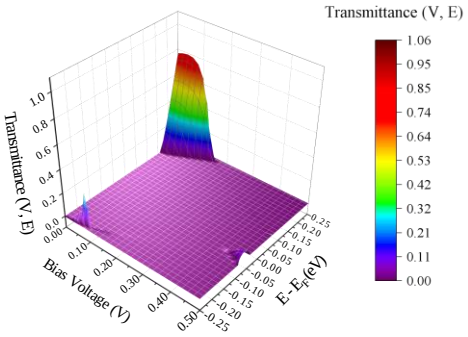

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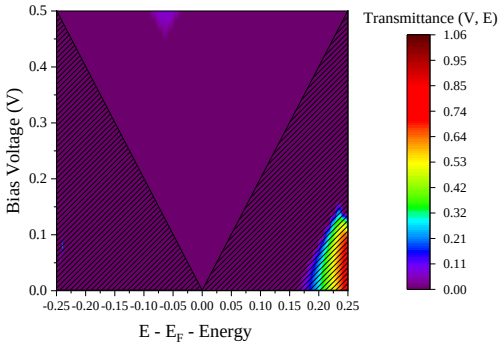

Figures: (a) Planar C-57; (b) Unit cell C-57; (c) Unit Cell C-57 Hydrogenated; (d) C-57 System; (e) C-57 hydrogenated system; (f) Current and conductance of the C-57 system; (g) Current and conductance of the hydrogenated system; (h) 3D and 2D density of states of C-57; (i) 3D and 2D density of states of hydrogenated; (j) 3D and 2D transmittance C-57; (l) 3D and 2D transmittance hydrogenated.

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