

Stacked Coronene Clusters on Graphene: DFT Insights into PAH Aggregation and Interstellar Infrared Bands

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Polycyclic aromatic hydrocarbons (PAHs) are widely recognized as key carriers of the Aromatic Infrared Bands (AIBs) observed across the interstellar medium [1]. Yet, the extent to which PAHs exist as isolated molecules or as π - π stacked clusters [2] and adsorbates on carbonaceous dust remains unresolved. Here, we use dispersion-corrected Density Functional Theory (DFT) and time-dependent DFT (TD-DFT) to investigate the structural and spectroscopic properties of coronene ($C_{24}H_{12}$) monomers, dimers (Figure 1), trimers, and tetramers as well as their adsorption on graphene-like carbon surface. Calculations at the ω B97X-D/def2-TZVP levels yield reliable binding and adsorption energies consistent with weakly bound, yet stable, aggregates under cold interstellar conditions (10–50 K). The computed IR spectra (3–20 μ m) reveal moderate redshifts, band broadening, and intensity redistribution - especially in the 6–9 μ m and 11–13 μ m regions-reproducing the plateau-like profiles in Spitzer and JWST observations. TD-DFT absorption spectra show minor redshifts and broadening of π - \rightarrow π^* transitions, supporting their possible link to diffuse interstellar bands.

These results indicate that stacked coronene clusters and PAH@graphene complexes could coexist with isolated PAHs, contributing to the observed diversity of interstellar IR emissions and bridging the molecular-to-grain transition in cosmic carbon chemistry.

References

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 - [2] M. Schmidt, A. Masson, C. Bréchnignac, *International Journal of Mass Spectrometry*, 252 (2006) 173–179.
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Figures

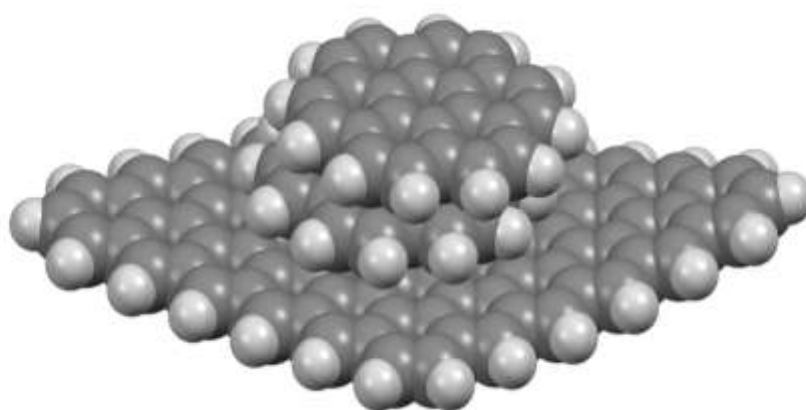


Figure 1: Coronene dimer adsorbed onto a graphene sheet. The optimized configuration illustrates π - π stacking interactions between planar aromatic coronene molecules and the graphene surface, suggesting possible multilayer aggregation relevant to interstellar PAH cluster formation.

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