Modelling Plasmon Excitations in Planar PAH Systems

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Synopsis We develop an analytical hydrodynamic model to investigate collective electronic excitations in PAH-inspired molecular systems. Using a jellium-based cylindrical shell geometry, we derive the bulk and surface charge-density modes, revealing multiple coupled surface plasmon branches arising from the system' s finite boundaries. This framework provides insight into the role of confinement and geometry in shaping molecular-scale collective excitations.

Collective excitations arise in a wide range of physical systems, from atomic nuclei, where they manifest as giant resonances such as the giant dipole resonance (GDR), to condensed-matter systems, where the coherent oscillations of delocalized electrons are known as plasmons [1–3]. These electronic excitations can couple strongly to electromagnetic radiation, giving rise to characteristic resonant responses. While plasmons are well established in bulk metals and metallic nanostructures, they have also been identified in finite carbon-based systems, including C60 fullerenes and polycyclic aromatic hydrocarbons (PAHs) [4, 5].

In PAHs, absorption features in the 17–18 eV energy range have been associated with molecular plasmon resonances, with reported absorption cross sections reaching 25 Mb–35 Mb per carbon atom [5]. The characteristics of these excitations depend on the size and topology of the molecule, motivating theoretical investigations of collective electronic behavior in finite, confined systems.

Plasmon resonances can be studied using different theoretical approaches, ranging from the classical Drude model to microscopic methods such as the random phase approximation (RPA) and time-dependent density functional theory (TDDFT) [6]. While these approaches describe collective electronic excitations at different levels of detail, their computational cost and treatment of nonlocal effects vary. The hydrodynamic model provides an intermediate approach, treating electrons as a continuous fluid while incorporating pressure effects and spatial dispersion [7]. In this work, we employ this model to investigate collective electronic excitations in planar molecular systems.

The model considers the system to be a finite cylindrical shell of electron gas within the jellium approximation, enabling the effects of confinement and boundary geometry to be treated analytically. Starting from the linearized hydrodynamic equations, we derive the governing equations for bulk and surface charge-density oscillations. The resulting formulation separates volume and boundary contributions to the induced charge density and yields a coupled set of equations for the surface modes. The model predicts a bulk plasmon mode at the characteristic plasma frequency, $\omega_p = \sqrt{4\pi\rho_0}$, alongside multiple coupled surface plasmon branches associated with the cylindrical and planar boundaries of the system.

This analytical framework provides a basis for investigating how confinement and boundary geometry shape collective electronic excitations in PAH-inspired molecular systems and related finite carbon nanostructures.

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