Physics Department
MSc Thesis Defense

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Collective Excitonic Modes in Materials with Hexagonal Carbon Rings

We investigate collective electronic modes in benzene, acenes (polyacenes), cyclacenes, and various forms of C_3N . These materials share a common structural motif—a hexagonal ring of carbon atoms, commonly known as the benzene ring. When benzene rings are connected in a one-dimensional edge-sharing arrangement, acenes are formed. Joining the ends of an acene results in a belt-like molecule called cyclacene. Arranging benzene rings in a two-dimensional plane, separated by nitrogen atoms, produces C_3N. To understand electron behavior, we first neglect interactions and employ a tight-binding description. We then introduce electron-electron interactions using the Hubbard model. These interactions generate internal fields that may combine with external fields, giving rise to resonances—oscillating patterns interpreted as collective modes studied by Random Phase Approximation method. A notable finding is the correlated oscillation of spins in benzene, polyacenes, and cyclacenes, which leads to the formation of dynamic anti-ferromagnets. Additionally, for all these materials, as the Hubbard interaction coefficient (U) increases, the frequency required for excitonic modes decreases. An increase in the number of benzene rings or layers of C_3N results in a decrease in the band gap size and frequencies. Tight-binding band structures for C_3N in monolayer and multilayer forms reveal that C_3N is a semiconductor. We observe the formation of excitons in monolayer C_3N with very low binding energy.