

Abstract Submitted
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Fullerene microcrystals under pressure¹ MURILO L. TIAGO, FERNANDO A. REBOREDO, Oak Ridge National Laboratory — Solid buckminsterfullerene (C_{60}) is known to be very soft, with a large number of crystalline phases that can be accessed by temperature or pressure. External pressure reduces the intermolecular distance, which affects the electronic structure in three ways: by increasing the overlap between molecular orbitals on neighbor molecules, by inducing additional chemical bonds between molecules, and by deforming the molecular structure. Having an exciton gap that is sensitive to pressure suggests that C_{60} can be used as active element in an optical pressure gauge: a device that can detect pressure dynamically on the material from the red-shift of its optical spectrum. Using first-principles many-body theories, we calculate the optical gap of solid C_{60} and its pressure dependence. We also analyze the dependence of optical gap with deformations in the molecule. Our calculations are based on solving the Bethe-Salpeter for electron-hole excitations. The electron self-energy is calculated within the GW approximation. We use pseudopotential density-functional theory to determine the electronic structure of C_{60} in its ground state.

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