AN ELECTRON DENSITY APPROACH TO UNDERSTAND HIGH-PRESSURE PHENOMENA

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Abstract

Pressure is a good thermodynamic variable to modify bond lengths and angles between the atomic constituents of crystals. Therefore, a microscopic study of the response of crystalline solids to increasing hydrostatic pressure provides a basic contribution to interpret and predict properties and behavior of materials. Formalisms of the analysis of the topology of the electron density reveal to be efficient theoretical tools to perform such a study. Some illustrative applications of these tools are proposed: (i) Decomposition of macroscopic compressibility in atomic, core and valence contributions, (ii) Verification of the so-called *anions in metallic matrices* model, and (iii) Visualization of chemical changes across solid-solid phase transitions