Ab Initio Studies of Pressure-Induced Structural and Electronic Changes in Inorganic Crystals

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Quantum mechanical study of the effects of pressure on crystal structures and their properties is one of the popular applications for density functional modeling. In this contribution, we will first discuss the reliability with which the structural response of crystals to applied pressure can be predicted. Quantum mechanical calculations also allow to investigate pressure-induced changes to the electronic structure.

The most obvious effects, such as pressure-induced metallization, and other large changes in the density of states and in the charge density distribution, can be monitored via the pressure dependence of the DOS and of the spatial distribution of the electron density.

These can be also analyzed as changes in bond populations, and thereby offer insight into the driving force of pressure-induced phase transitions. This is especially interesting for iso-symmetric structural phase transitions, where small structural changes give rise to first-order transitions. Furthermore, changes in hydrogen bonding under pressure and pressure-induced charge-disordering can reliably be investigated.