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Deductive Quantum Molecular Mechanics of Carbon Allotropes

Initiative: Trilaterale Partnerschaften – Kooperationsvorhaben zwischen Wissenschaftler(inne)n aus der

Ukraine, Russland und Deutschland

Bewilligung: 28.02.2016

Laufzeit: 2 Jahre

Projekt-Website: www.ssc.rwth-aachen.de

It is proposed to develop an alternative deductive quantum molecular mechanics approach which directly reflects the chemical bonds by a thorough analysis of the local electronic structure, namely by the hybridization of the involved atomic orbitals, the bonding pattern, and the bond strain. Alternatively expressed, such general analysis yields an allotrope's total energy as an explicit function of its spatial structure (interatomic separations) and of the orientations and forms of the hybrid atomic orbitals (that is, the hybridization tetrahedra) residing on the carbon atoms. By doing so, the total energy may be mechanistically and, hence, locally interpreted, namely that of a system composed of moving and rotating flexible tetrahedra. Their interactions are derived from the architecture of the allotrope's many-electron wave function as reflected by the bonding pattern, i.e., from the assembly of either two-center s- or p-bonds or topology-specific wave functions describing conjugated p-electrons. This newly developed and supposedly ultrafast theory will be implemented as a stand alone code. The first tests will be carried out against the experimental data available for known allotropes and also reliable DFT data for hypothetical ones. Second, the new theory will be applied to analyze or predict the hardness of unusual carbon allotropes, and it will be made available to the entire scientific community to numerically rank the variety of carbon networks. Third, the new method will also be utilized to access the electronic structure and mechanical properties of amorphous carbon often suggested as a perspective construction material.

Projektbeteiligte

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