

Computer simulations of polymorphic carbon, 'as good as it gets'.

A. Fasolino

Institute for Molecules and Materials, Radboud University Nijmegen

Carbon is maybe the most versatile element in the periodic table. It occurs in nature in forms with very different, and often exceptional, physical properties, from diamond and graphite to fullerenes, nanotubes and the recently discovered graphene. The interest in carbon structures spans many different fields, from material science to electronics and geophysics.

Computer simulations play a very important role in the characterization of existing carbon materials, also in extreme conditions, and in the search for new carbon structures. However, the multiplicity of types of bonding makes simulations of carbon materials very challenging. We have developed the reactive phenomenological bond order potential LCBOP (J.Los et al, Phys. Rev B 72,214102 (2005)), suitable for large scale simulations.

In this talk I will discuss the merits of our approach for the description of the structural properties and transformations of carbon, while presenting the calculated liquid, diamond, graphite phase diagram. I will close by presenting some very recent results for single and double layer graphene.

