Structural *map* of elemental Carbon

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Carbon and carbon-based materials are of great importance for different applications, such as electronic devices, hard materials, hydrogen storage etc. The large variety of properties found in carbon structures is connected to the polymorphism which is a direct consequence of the flexible C-C (sp^1-sp^2-sp^3) bonding [1]. The large number of possible allotropes pose challenges in structural nomenclature, identification and classification, which has been hardly addressed properly till date [2]. In this work we address the issue of structural classification of 3D periodic structures, generated with the Minima Hopping Method [3], which is a flexible and powerful method to find low-energy structures for a generic chemical composition. Based on the analysis of the bonding pattern and the local atomic arrangement of our structural candidates, we developed a structural map of carbon, classifying them in three families : (i) Graphite-like, (ii) Diamond-like and (iii) Tubulanes. Tubulanes are characterised by mixed sp^1-sp^2-sp^3 bonding and can be visualised as a 3D parallel network of tube-like structures. These tubular structures display a wide range of electronic properties i.e. metal, insulator and semimetal. Few of the tubulane structures are found to exhibit non-trivial topological properties.

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