



Computer-Based Modeling of Novel Carbon Systems and Their Properties: Beyond Nanotubes (Carbon Materials: Chemistry and Physics)

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During the last twenty years, the multiplicity of potential carbon structures has consistently posed a formidable challenge to theoretical and computational physicists. Several different methods are currently being used to study the structure and the properties of such systems. These methods include simulations based on empirical potentials, tight-binding calculations and density functional theory (DFT). A combination of these methods is needed to make significant progress in the carbon field.

This volume provides the reader with a survey of state-of-the-art theoretical and computational contributions featuring novel carbon systems (excluding nanotubes). The chapters are authored by leading researchers who are all actively involved with different aspects of carbon structure and property elucidation. Consequently, a variety of methods are presented to the reader. The editors have successfully compiled an informative book that:

- Showcases the latest results in carbon materials
- Demonstrates how different theoretical methods are combined
- Explains how new carbon structures are predicted

Computer-Based Modeling of Novel Carbon Systems and Their Properties is aimed at advanced undergraduates, graduates, and researchers with an interest in computational nanomaterials.

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