

Computational Physics Of Carbon Nanotubes



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Carbon nanotubes are the fabric of nanotechnology. Investigation into their properties has become one of the most active fields of modern research. This book presents the key computational modelling and numerical simulation tools to investigate carbon nanotube characteristics.

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4 Interatomic potentials and force-fields in the computational physics of carbon nanotubes 4.1 Interatomic potential energy function (PEF) 4.2 Force-field (molecular mechanics) method 4.3 Energetics of carbon nanotubes 4.4 Energetics of SWCNT-C60 and C60-C60 interactions 4.5 Energetics of fluid flow through carbon nanotubes

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The physics of carbon nanotubes is intimately bound up with the emerging and exciting fields of computational nano-science, computational nano-technology, computational materials science and computational condensed matter physics.

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