

Quantum Chemical Modeling of the Complexes of Squaraine Dyes with Carbon Nanoparticles: Graphene, Nanotube, Fullerene

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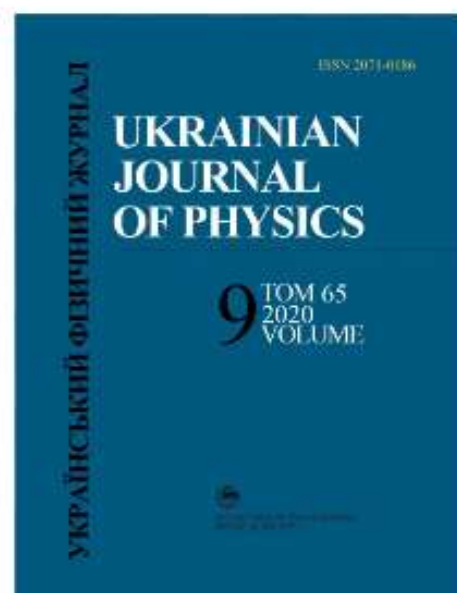
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Abstract

The geometry and electronic structure of the complexes of dyes containing various numbers of electron-donor oxygen atoms and carbon nanostructures with various dimensions (fullerene C_{60} , carbon nanotube, graphene) have been studied. It is shown that the charge transfer from the dyes to the carbon nanostructures leads to changes in the geometry of carbon nanostructures and the dye chromophores, as well as in the electronic structure of the whole complexes.



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