

TDDFT for nanostructures and biomolecules

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Reviews

An exceptional book and also the font utilized was intriguing to read. This is for all who statte there was not a worth reading. It is extremely difficult to leave it before concluding, once you begin to read the book. (Prof. Tyson Hilpert)

TDDFT FOR NANOSTRUCTURES AND BIOMOLECULES



Condition: New. Publisher/Verlag: LAP Lambert Academic Publishing | A time-dependent density-functional theory scheme for the computation of the electromagnetic response of nanostructure | We present a study of first principles computational techniques for the description of chemical systems in the nanometer scale: clusters, nanostructures and biomolecules. The scope of our methodology comprises linear and non-linear interactions of electromagnetic fields with nanostructures, the latter being described through the point-nuclei approximation, whereas the electromagnetic fields are described classically. We have focused on both small to medium sized inorganic clusters and on small organic and biological systems. We have considered both their linear photoresponse (e.g. optical absorption) and their non-linear interaction with intense femtosecond lasers. Also, the underlying nuclear structure is not inert: the coupling of the excited electronic states with the vibronic degrees of freedom is also studied --- which may lead to processes such as photodissociation, photoisomerization, etc. In these latter cases, we have investigated non-adiabatic molecular dynamics simulations within our formalism. | Format: Paperback | Language/Sprache: english | 367 gr | 220x150x14 mm | 264 pp.

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