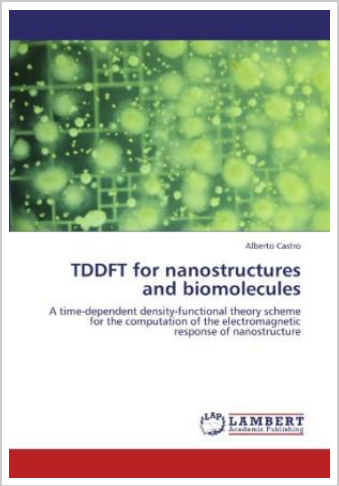

DOWNLOAD

TDDFT for nanostructures and biomolecules

By Castro, Alberto

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.

READ ONLINE
[4.88 MB]

Reviews

It in a of the most popular publication. It is actually rally intriguing throgh looking at time period. Your daily life span is going to be change the instant you total reading this publication.

-- ***Mrs. Shanna Mann***

Totally among the best publication I have ever go through. This really is for all those who statte that there had not been a well worth studying. I am just very happy to let you know that this is actually the very best pdf we have go through inside my very own daily life and could be he very best ebook for actually.

-- ***Miss Audra Moen***