



## 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**  
[ 1.03 MB ]

### Reviews

*This book is definitely not straightforward to get started on studying but extremely exciting to read. It is really simplistic but shocks in the 50 percent of the ebook. Once you begin to read the book, it is extremely difficult to leave it before concluding.*

-- **Ally Reichel**

*This publication is amazing. It is definitely basic but shocks in the fifty percent of your publication. You wont feel monotony at anytime of your own time (that's what catalogues are for concerning if you question me).*

-- **Prof. Kirk Cruickshank DDS**

## Other PDFs

---



### **All New Kindle Fire HD Complete Guide for Seniors: How to Get the Most Out of Your Kindle Devices with Simple Step-By Step Instructions in 30 Minutes. (Paperback)**

Createspace Independent Publishing Platform, 2017. Paperback. Condition: New. Language: English . Brand New Book \*\*\*\*\* Print on Demand \*\*\*\*\*. Are you looking for a kindle fire HD guide that could help you get the most out of your device? Whether you own...

---



### **INTERNATIONAL EDITION---Marketing: Real People, Real Choices, 8th edition**

Paperback. Condition: New. INTERNATIONAL EDITION, brand New, International/Global Edition, NOT LOOSE LEAF VERSION, NO SOLUTION MANUAL, NO CD, NO ACCESS CARD, Soft Cover/ Paper Back written in English, Different ISBN and Cover Image from US Edition; Sometimes, the title is different from US...

---



### **Autodesk Revit 2016 MEP Fundamentals (Ascent) (Paperback)**

SDC Publications, United States, 2016. Paperback. Condition: New. Language: English . Brand New Book. To take full advantage of Building Information Modeling, the Autodesk Revit 2016 MEP Fundamentals has been designed to teach the concepts and principles of creating 3D parametric models...

---



### **Kurenai the Crimson 1865: An Oiran, a Ninja and a Hiding Christian (Paperback)**

Createspace, United States, 2014. Paperback. Condition: New. Language: English . Brand New Book \*\*\*\*\* Print on Demand \*\*\*\*\*. Beautiful Kurenai is an oiran, the highest level of a geisha. Though she now lives in splendor, she came from poverty. And when a millionaire...

---



### **Kindred Souls**

Katherine Tegen Books. Paperback. Condition: New. New copy - Usually dispatched within 2 working days.

---



### **Kindred**

2012. PAP. Condition: New. New Book. Shipped from US within 10 to 14 business days. Established seller since 2000.

---