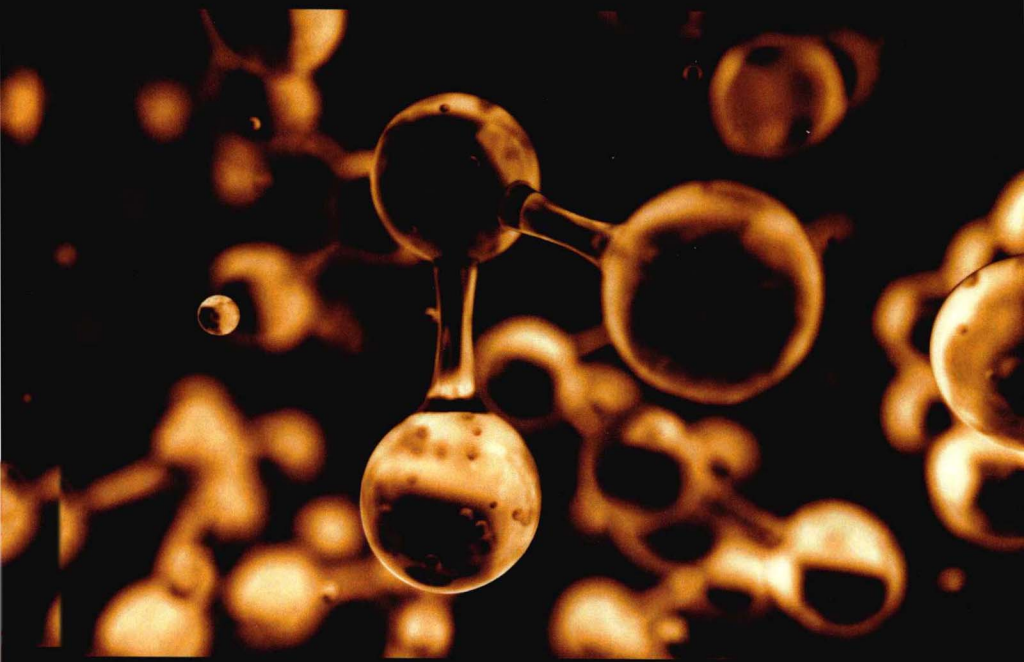
Computational Chemistry Methodology in Structural Biology and Materials Sciences

Editors
Tanmoy Chakraborty | Prabhat Ranjan | Anand Pandey



AAP APPLE ACADEMIC PRESS

CRC Press
Taylor & Francis Group

COMPUTATIONAL CHEMISTRY METHODOLOGY IN STRUCTURAL BIOLOGY AND MATERIALS SCIENCES

Edited by
Tanmoy Chakraborty, PhD
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Apple Academic Press Inc.
3333 Mistwell Crescent
Oakville, ON L6L 0A2 Canada

Apple Academic Press Inc.
9 Spinnaker Way
Waretown, NJ 08758 USA

Printed in the United States of America on acid-free paper
International Standard Book Number-13: 978-1-77188-568-3 (Hardcover)
International Standard Book Number-13: 978-1-315-20754-4 (eBook)

Library and Archives Canada Cataloguing in Publication

Computational chemistry methodology in structural biology and materials sciences / edited by Tanmoy Chakraborty, PhD, Prabhat Ranjan, BE, MTech, Anand Pandey, PhD.

Includes bibliographical references and index.
Issued in print and electronic formats.
ISBN 978-1-77188-568-3 (hardcover).--ISBN 978-1-315-20754-4 (PDF)

1. Chemistry, Physical and theoretical--Data processing. 2. Chemistry, Physical and theoretical--Methodology. 3. Biology. 4. Materials science. I. Chakraborty, Tanmoy, editor II. Ranjan, Prabhat (Mechatronics professor), editor III. Pandey, Anand, editor

QD455.3.E4C66 2017 541.0285 C2017-903269-0 C2017-903270-4

Library of Congress Cataloging-in-Publication Data

Names: Chakraborty, Tanmoy, editor. | Ranjan, Prabhat, (Mechatronics professor) editor. | Pandey, Anand, editor.
Title: Computational chemistry methodology in structural biology and materials sciences / editors, Tanmoy Chakraborty, PhD, Prabhat Ranjan, BE, MTech, Anand Pandey, PhD.
Description: Toronto; New Jersey: Apple Academic Press, 2017. | Includes bibliographical references and index.
Identifiers: LCCN 2017021264 (print) | LCCN 2017028825 (ebook) | ISBN 9781315207544 (ebook) | ISBN 9781771885683 (hardcover : alk. paper)
Subjects: LCSH: Proteins--Structure--Mathematical models. | Materials science--Mathematical models. | Chemistry--Electronic data processing.
Classification: LCC QP551 (ebook) | LCC QP551 .C7124 2017 (print) | DDC 572/.633--dc23
LC record available at https://lccn.loc.gov/2017021264

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LIST OF ABBREVIATIONS

4hC	4-hydroxy coumarin
4mE	4-methyl esculetin
7h4mC	7-hydroxy-4-methyl coumarin
7hC	7-hydroxy coumarin
ADME	absorption, distribution, metabolism and excretion
BLYP	Becke-Lee-Yang-Parr
BSSE	basis set superposition error
C	coumarin
CFs	core functions
CI	cyberinfrastructures
CIS	configuration interaction singles
COs	core orbitals
CP	critical point
CPCM	conductor-like polarizable continuum model
CT	charge transfer
DA	dissociative adsorption
DBs	discrete breathers
DC	3,4-dihydrocoumarin
DCA	dichloroacetate
DFT	density functional theory
DOS	density of states
DSSC	dye sensitized solar cells
E	esculetin
EA	electron affinity
EGI	European grid infrastructure
EM	electromagnetic
EMM	molecular mechanics energies
Evdw	van der Waals interactions
FDTD	finite difference-time domain
FFs	force fields
FWHM	full width at half-widths maximum

GGA	generalized gradient approximation
HOMO	highest occupied molecular orbital
HPC	high-performance computer
IC	internal coordinates
ILM	intrinsic localized modes
IP	ionization potential
KB	Kleinman and Bylander
LCPO	linear combination of pairwise overlaps
LIA	linear interaction approximation
LOB	large object datatypes
LP	lone pair
LUMO	lowest unoccupied molecular orbitals
MB	Maxwell-Bloch
MC	Monte Carlo
MD	molecular dynamics
MI	magneto-inductive
MM	molecular mechanics
MM	metamaterial
NBO	natural bond orbital
NCPPs	norm-conserving pseudo potentials
NIR	near infra-red
NLKG	nonlinear Klein-Gordon
NLO	nonlinear optical
NLSE	nonlinear Schrodinger equation
NMODE	normal mode
NPA	natural population analysis
NSF	National Science Foundation
OFETs	organic field effect transistors
OLEDs	organic light emitting diodes
OPVs	organic photovoltaic cells
OSC	organic solar cell concentrators
P	polarization
PAW	projected augmented wave
PBC	periodic boundary conditions
PBS	portable batch system
PCM	polarizable continuum model

PDC	pyruvate dehydrogenase complex
PDE	partial differential equations
PDHK	pyruvate dehydrogenase kinase
PDOS	partial density of states
PEN	pentacene
PP	pseudopotential
PSA	polar surface area
pWT	phosphoSer768 wild-type
QBs	quantum breathers
QM	quantum mechanics
QNPC	quadratic nonlinear photonic crystal
QPM	quasi-phase matching
RCSB	Research Collaboratory for Structural Bioinformatics
RIC	redundant internal coordinates
RLC	resistor-inductor-capacitor
RMSD	root-mean square deviation
RR	Resonance Raman
S	Softness
SBH	Schottky barrier height
SCF	similar convergence
SCF	self-consistent field
SFOs	symmetrized fragment orbitals
SGB	surface generalized born
SHG	second harmonic generation
SRR	split-ring-resonators
TD-DFT	time dependent density functional theory
TET	targeted energy transfer
TM	transmembrane
TPA	triphenylamine
TPBS	two-phonon bound state
TPSA	topological PSA
TRPC	transient receptor potential-canonical
TRPC6	transient receptor potential-canonical-6
TS	transition state
UPML	uniaxial perfectly matched layer
vdW	van der Waals

VPAC	Victorian Partnership for Advanced Computing
VRM	virtual reality modeling
XP	extra precision
XSEDE	Extreme Science and Engineering Discovery Environment

PREFACE

This book, *Computational Chemistry Methodology in Structural Biology and Material Sciences*, provides a survey of research problems in theoretical and experimental chemistry. The subject matter covered in the book varies from materials science to biological activity. Part 1 of the book emphasizes new developments in the domain of theoretical and computational chemistry and its applications to bio-active molecules, whereas in Part 2 the study of materials science has been depicted vividly.

In Chapter 1, the authors have computed the pK_a value of a number of alkylamines using the density functional theory (DFT) methodology. Considering versatility and importance of amines in different domain, this particular study is very useful and relevant. It will help to explain the mechanistic feature of CO_2 capturing processes by amines. A close agreement is observed between experimental parameters with the computed data.

Keeping in view the wide biological importance of coumarins, this report is very useful. The study on the effects of unsaturation of chemical reactivity of coumarins has been reported in Chapter 2. Invoking DFT-based descriptors, the authors have shown the reactivity variations by substitution. Site selectivity has been also predicted by using local DFT-based descriptors.

In Chapter 3, molecular dynamics simulations have been utilized to study the interaction between FKBP12 (FK506 binding protein-12 kDa) and transient receptor potential-canonical 6 (TRPC6). The computed data have identified thermodynamically favorable binding affinity with FKBP12. The study reveals the formation of specific binding pockets for the recognition and interaction of FKBP12 with the TRPC6 intracellular domain.

In Chapter 4, the author has worked on finding inhibitors of the pyruvate dehydrogenase kinase (PDHK). He has explored the interaction within dichloroacetate (DCA) and PDHK2. The results of virtual screening are

in similar line with the experimental findings. A search for more potent inhibitors is discussed.

The evolution of computational chemistry is mapped in this report. Two parallel approaches of computational chemistry viz. quantum mechanics and molecular mechanics have been discussed. The importance of two approaches, different computational techniques, and latest development has been noted in Chapter 5.

The application of computational chemistry to design new materials is nicely reflected in Chapter 6. Designing of photoactive materials is an active field of research. In this report, computational processes for designing and modeling of photoactive compounds having application in the solar cells are reported. The unique features of dye-sensitized solar cells have been studied in terms of computational processes, and predictions have been done toward new photovoltaic materials in terms of modeling.

In Chapter 7, the authors have tried to predict stable adsorption geometry of organic molecule on metal surface invoking using theoretical technique. Some of electronic properties have been considered to characterize charge transfer properties of organic molecules.

In Chapter 8, the conversion of methane to liquid fuels in terms of DFT has been reported. C-H bond activation of methane promoted by Pt and Pd sub-nanoclusters have been investigated and reported. The study reveals the efficacy of Pt clusters in breaking of C-H bond in methane.

In Chapter 9, the electronic, magnetic and optical properties of copper-silver nano alloy clusters have been studied in terms of DFT-based descriptors in this analysis. Computed DFT descriptors nicely correlate the optical properties of instant compound. Theoretical parameters show a hand-in-hand trend with experimental data.

In Chapter 10, the authors have derived nonlinear Klein Gordon-equation for metamaterials in terms of the model behavior of split-ring resonators for the application in antenna. The variation principle has been applied to reach mathematical equations. Multisolitone behavior of metamaterial system has also been explained by this work.

In Chapter 11, the model has been developed for dispersive active materials in finite-difference time-domain (FDTD) framework. The dispersive materials having optical properties have been modeled in terms of relative dielectric permittivity. A second-order optimized algorithm has

been used to deal with the dispersion. In addition, there is a discussion of the Maxwell-Bloch (MB) formalism and solution.

In Chapter 12, a synthesizing technique of nanocrystalline AlMgFeCu-CrNi has been discussed. Experimental technique successfully predicts the behaviors of the synthesize compounds. The phase transfer observation is also discussed.

Overall, this book, *Computational Chemistry Methodology in Structural Biology and Material Sciences*, is a collection of chapters that cover a wide range of subject matter regarding the application of theoretical and experimental chemistry, materials science, and biological domain. The research present in this book is very important in the context of contemporary research problems.

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Tanmoy Chakraborty, PhD, is Associate Professor in the Department of Chemistry at Manipal University Jaipur, India. He has been working in the challenging field of computational and theoretical chemistry for the last six years. He has completed his PhD from the University of Kalyani, West-Bengal, India, in the field of application of QSAR/QSPR methodology in the bioactive molecules. He has published many international research papers in peer-reviewed international journals with high impact factors. Dr. Chakraborty is serving as an international editorial board member of the *International Journal of Chemoinformatics and Chemical Engineering*. He is also reviewer of the *World Journal of Condensed Matter Physics* (WJCMP). Dr. Tanmoy Chakraborty is the recipient of prestigious Parameswar Mallik Smawarak Padak, from Hooghly Mohsin College, Chinsurah (University of Burdwan), in 2002.

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