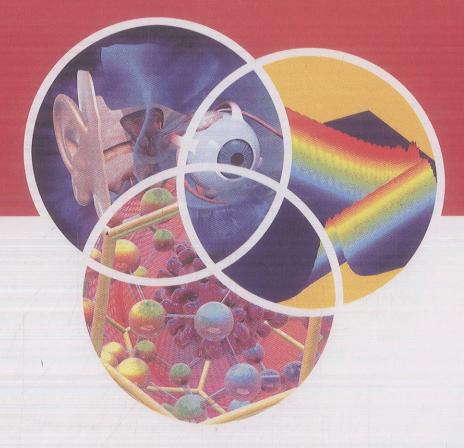
Computational Studies New Materials II

From Ultrafast Processes and Nanostructures to Optoelectronics, Energy Storage and Nanomedicine



Thomas F George • Daniel Jelski Renat R Letfullin • Guoping Zhang

editors



Contents

Preface List of Contributors Introduction Thomas F. George, Daniel Jelski, Renat R. Letfullin and Guoping Zhang		v xi xix			
			1.	Laser-Matter Interactions: Nanostructures, Fabrication and Characterization László Nánai, Zsolt I. Benkő, Renat R. Letfullin and Thomas F. George	1
			2.	Nanoscale Materials in Strong Ultrashort Laser Fields Renat R. Letfullin and Thomas F. George	37
3.	Exciting Infrared Normal Modes in C ₆₀ by an Ultrafast Laser Guoping Zhang and Thomas F. George	65			
4.	Self-Interaction-Free Time-Dependent Density Functional Theoretical Approaches for Probing Atomic and Molecular Multiphoton Processes in Intense Ultrashort Laser Fields Shih-I Chu and Dmitry Telnov	75			
5.	Nanomaterials in Nanomedicine Renat R. Letfullin and Thomas F. George	103			

6.	New Dynamic Modes for Selective Laser Cancer Nanotherapy	131
	Renat R. Letfullin and Thomas F. George	
7.	New Direct Inhibitors and Their Computed Effect on the Dynamics of Thrombin Formation in Blood Coagulation Liliana Braescu, Marius Leretter and Thomas F. George	173
8.	Laser Ablation of Biological Tissue by Short and Ultrashort Pulses Renat R. Letfullin and Thomas F. George	191
9.	Incorporating Protein Flexibility in Molecular Docking by Molecular Dynamics: Applications to Protein Kinase and Phosphatase Systems Zunnan Huang and Chung F. Wong	219
10.	Spin Valves in Conjugated Polymeric Light-Emitting Diodes Sheng Li, Guo-Ping Tong and Thomas F. George	251
11.	Optical Properties of Wurtzite ZnO-Based Quantum Well Structures with Piezoelectric and Spontaneous Polarizations Seoung-Hwan Park, Doyeol Ahn, Sam Nyung Yi, Tae Won Kang and Seung Joo Lee	273
12.	Tailoring Electronic and Optical Properties of TiO ₂ : Nanostructuring, Doping and Molecular-Oxide Interactions Letizia Chiodo, Juan Maria Garciá-Lastra, Duncan John Mowbray, Amilcare Iacomino and Angel Rubio	301

13.	Computational Studies of Tailored Negative-Index Metamaterials and Microdevices Alexander K. Popov and Thomas F. George	331
14.	Nanoscale Resolution in the Near and Far Field Intensity Profile of Optical Dipole Radiation Xin Li, Henk F. Arnoldus and Jie Shu	379
15.	Laser-Induced Femtosecond Magnetism Guoping Zhang and Thomas F. George	405
16.	Gas-Dispersed Materials as an Active Medium of Chemical Lasers Renat R. Letfullin and Thomas F. George	423
17.	Transport Coefficients in ³ He- ⁴ He Mixtures Sahng-Kyoon Yoo, Chung-In Um and Thomas F. George	451
18.	Computational Discovery of New Hydrogen Storage Compounds Eric Majzoub	481
Inde	Index	
About the Editors		511