

# Computational Studies *of* New Materials II

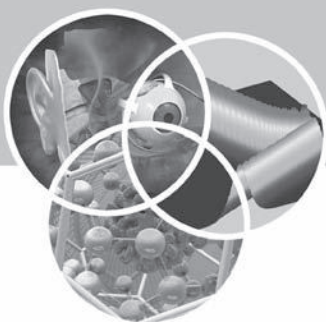
From Ultrafast Processes and Nanostructures to  
Optoelectronics, Energy Storage and Nanomedicine



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

*editors*

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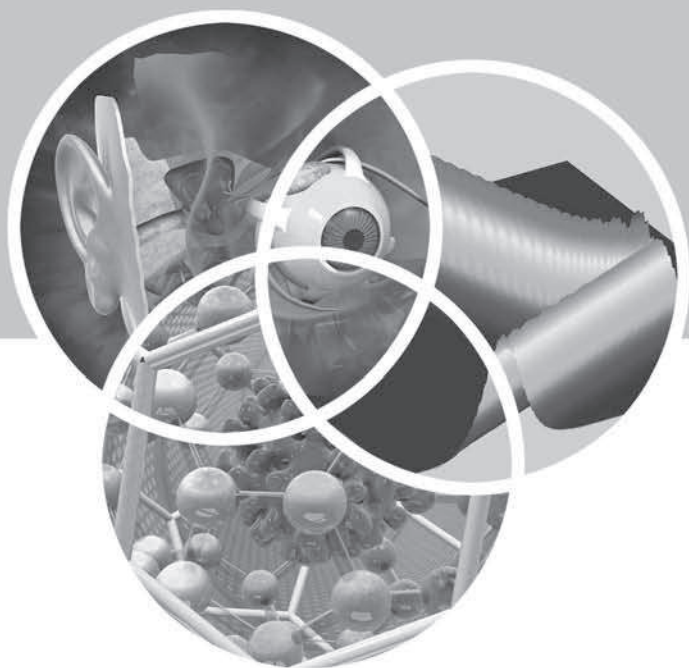


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From Ultrafast Processes and Nanostructures to Optoelectronics,  
Energy Storage and Nanomedicine**

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## Preface

In 1999 at the request of World Scientific, Daniel Jelski and Thomas F. George edited a book entitled *Computational Studies of New Materials* consisting of fourteen chapters written by leading experts on topics including fullerenes, semiconductors, fractals, polymers and nonlinear optical processes. In 2008, Dr. Zvi Ruder, senior executive editor at World Scientific, approached us about editing a sequel, or second volume. We agreed to this venture with two additional editors — Renat R. Letfullin and Guoping Zhang — and decided upon the title *Computational Studies of New Materials II*.

While the 1999 book was quite timely when it was published, much has evolved during the past decade in the development of new materials and appropriate computational techniques, especially with the “explosion” of interest and activity in nanoscience and nanotechnology. It is worth noting that the stage was set for this from a federal perspective when in 1999 US President Bill Clinton’s science advisor, Neal Lane, rated nanotechnology as one of the government’s 11 inter-agency R&D priorities for the purpose of planning the FY 2001 budget.<sup>a</sup>

Nanomaterials, i.e., materials with dimensions on the scale of a nanometer, play a prominent role in this current 2010 book. This includes ultrafast processes stimulated by short laser pulses, such as in connection with fullerenes, and the exciting field of nanomedicine, such as selective laser cancer therapy using gold nanospheres and nanorods. Topics in addition to nanomaterials include energy storage and optoelectronics, such as in connection with polymeric light-emitting

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<sup>a</sup> *OE Reports*, Number **188** (Society of Photo-Optical Instrumentation Engineers, August 1999).

diodes, semiconductor quantum wells, and tailored negative-index metamaterials and microdevices.

We ourselves have authored a number of the chapters and have invited various outstanding scientists throughout the world to serve as chapter authors. We are most impressed by the extremely high caliber of research and its presentation in the chapters by our colleague contributors. We thank the staff in the chancellor's office at UM–St. Louis for their help throughout the editorial process. We also thank Ms. Hwee Yun Tan (editor) and Ms. Jen Nie Kasim (marketing) at World Scientific for their role in producing and promoting this book.

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

March 2010

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### **In the world of science, ten years is a very long time!**

Back in 1999, World Scientific published a volume entitled *Computational Studies of New Materials* [1] for which two of us served as the editors. A decade later, we were approached by World Scientific about editing a second volume. Adding two more editors, the four of us discussed the relationship between the first volume and this current second volume. Has the world changed so much that we need a new title? Or is this a continuation of what was done before?

This is, after all, a Rip Van Winkle experience. It's as if we had gone to sleep for ten years and awoke to find the world a completely different place. The original title was carefully chosen, where the emphasis was on the materials, and less on the computational algorithms. New materials in