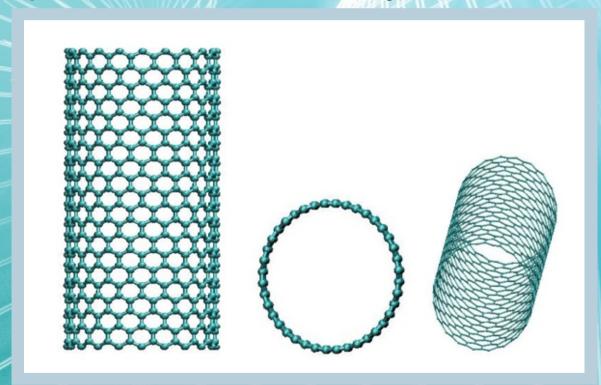
ISSN: 2153-1196 Vol. 5, No. 4, February 2014



# Journal of Modern Physics

# Special Issue on Molecular Dynamics Method





# **Journal Editorial Board**

ISSN: 2153-1196 (Print) ISSN: 2153-120X (Online)

http://www.scirp.org/journal/jmp

# **Editors-in-Chief**

Prof. Moshe Gai University of Connecticut, USA

Prof. Yang-Hui He City University, UK

# **Executive Editor-in-Chief**

Prof. Marko Markov Research International, Buffalo Office, USA

# **Editorial Board**

**Prof. Yohannes Abate**California State University, USA

Dr. Mohamed Abu-Shady Department of Applied Mathematics, Menoufia University, Egypt

Prof. Sadhan Kumar AdhikariUniversidade Estadual Paulista, BrazilDr. Hamid AlemohammadAdvanced Test and Automation Inc., CanadaDr. Ksenofontov AlexandreMoscow Engineering Physics Institute, RussiaProf. Sami M. AL-JaberAn-Najah National University, Palestine

Prof. Kerim R. Allakhverdiev Institute of Physics, Azerbaijan Academy of Sciences, Azerbaijan

Prof. Roberto Oscar AquilanoUniversidad Nacional de Rosario, ArgentinaDr. Salvatore CapozzielloUniversity of Naples Federico II, ItalyProf. Riccardo CerulliGran Sasso National Laboratory, INFN, Italy

Prof. Changle Chen

Celanese Corporation, USA
Prof. Stephen Robert Cotanch

NC State University, USA

Prof. Papadopoulos Demetrios

Aristotle University of Thessaloniki, Greece
Prof. Hugghy Doy

Theirang Sci. Tech University, China

Prof. Huashu Dou Zhejiang Sci-Tech University, China

Prof. Constantin Fetecau Gheorghe Asachi Technical University of Iasi, Romania

Prof. Ju GaoThe University of Hong Kong, ChinaProf. Sachin GoyalUniversity of Michigan, USADr. Wei GuoFlorida State University, USADr. Alioscia HammaTsinghua University, ChinaDr. Guangjin HouUniversity of Delaware, USA

Prof. Cosmin Ilie
Los Alamos National Laboratory, USA
Prof. Preston B. Landon
Prof. Chunlei Liu
Carnegie Mellon University, USA
Dr. Ray Luo
University of California, USA
University of California, USA

Prof. Karo Michaelian National Autonomous University of Mexico, Mexico

Prof. Karo Michaelian

Prof. Christophe J. Muller

Prof. Zdzislaw E. Musielak

Prof. Ambarish Nag

Prof. Luciano Nunziante

Prof. Valery Obukhov

National Renewable Energy Laboratory, USA

University of Naples Federico II, Italy

Tomsk State Pedagogical University, Russia

Prof. Valery Obukhov

Dr. Jorge Pereira

Prof. Tongfei Qi

Prof. Richard Saurel

Tomsk State Pedagogical University,
The University of Notre Dame, USA
University of Kentucky, USA
University of Aix Marseille I, France

Prof. Alejandro Crespo Sosa Universidad Nacional Autónoma de México, Mexico

Dr. Bo Sun
Princeton University, USA
Prof. Mingzhai Sun
Ohio State University, USA
Dr. Sergei K. Suslov
Arizona State University, USA
Academy of Finland, Finland

Dr. A. L. Roy Vellaisamy

Prof. Yuan Wang

Academy of Finland, Finland

City University of Hong Kong, China

University of California, Berkeley, USA

Prof. Magnus Willander Linköping University, Sweden

Prof. Fan Yang Fermi National Accelerator Laboratory, USA

Prof. Peter H. YoonUniversity of Maryland, USADr. S. ZerbiniUniversity of Trento, Italy

Prof. Meishan Zhao James Frank Institute, University of Chicago, USA
Prof. Pavel Zhurayley University of Maryland at College Park, USA

# **Managing Executive Editor**

Prof. Chang Liu Wuhan University, China Email: cliu@acc-lab.whu.edu.cn



# Call for Papers

# Journal of Modern Physics

http://www.scirp.org/journal/jmp

**Journal of Modern Physics (JMP)** is an international journal dedicated to the latest advancement of modern physics. The goal of this journal is to provide a platform for scientists and academicians all over the world to promote, share, and discuss various new issues and developments in different areas of modern physics.

# **Editors-in-Chief**

Prof. Moshe Gai University of Connecticut, USA

Prof. Yang-Hui He City University, UK

# **Executive Editor-in-Chief**

Prof. Marko Markov Research International, Buffalo Office, USA

# **Subject Coverage**

Journal of Modern Physics publishes original papers including but not limited to the following fields:

Biophysics and Medical Physics Complex Systems Physics Computational Physics Condensed Matter Physics Cosmology and Early Universe Earth and Planetary Sciences General Relativity High Energy Astrophysics High Energy/Accelerator Physics Instrumentation and Measurement Interdisciplinary Physics

Materials Sciences and Technology Mathematical Physics Mechanical Response of Solids and Structures New Materials: Micro and Nano-Mechanics and Homogeneization Non-Equilibrium Thermodynamics and Statistical Mechanics Nuclear Science and Engineering Optics Physics of Nanostructures

Plasma Physics
Quantum Mechanical Developments
Quantum Theory
Relativistic Astrophysics
String Theory

Superconducting Physics Theoretical High Energy Physics

Thermology

We are also interested in: 1) Short Reports—2-5 page papers where an author can either present an idea with theoretical background but has not yet completed the research needed for a complete paper or preliminary data; 2) Book Reviews—Comments and critiques.

# **Notes for Intending Authors**

Submitted papers should not have been previously published nor be currently under consideration for publication elsewhere. Paper submission will be handled electronically through the website. All papers are refereed through a peer review process. For more details about the submissions, please access the website.

# Website and E-Mail

http://www.scirp.org/journal/jmp E-mail: jmp@scirp.org

# What is SCIRP?

Scientific Research Publishing (SCIRP) is one of the largest Open Access journal publishers. It is currently publishing more than 200 open access, online, peer-reviewed journals covering a wide range of academic disciplines. SCIRP serves the worldwide academic communities and contributes to the progress and application of science, by delivering superior scientific publications and scientific information solution provider that enable advancement in scientific research.

# What is Open Access?

All original research papers published by SCIRP are made freely and permanently accessible online immediately upon publication. To be able to provide open access journals, SCIRP defrays operation costs from authors and subscription charges only for its printed version. Open access publishing allows an immediate, world-wide, barrier-free, open access to the full text of research papers, which is in the best interests of the scientific community.

- •High visibility for maximum global exposure with open access publishing model
- •Rigorous peer review of research papers
- Prompt faster publication with less cost
- •Guaranteed targeted, multidisciplinary audience





Website: http://www.scirp.org Subscription: sub@scirp.org Advertisement: service@scirp.org



# **TABLE OF CONTENTS**

Volume 5	Number 4	February 2014
·	vnamics Simulations of the DNA-CNT Interaction Process: Hyl	brid Quantum Chemistry
Potential and	Classical Trajectory Approach	
M. A. Khusen	ov, E. B. Dushanov, K. T. Kholmurodov	137
<b>Future Theor</b>	retical Approaches in Nuclear Magnetic Resonance	
E. S. Mananga	a	145
Spectral Mod	lifications of Graphene Using Molecular Dynamics Simulations	S
D Liesegang	C Olioschleger	149

The figure on the front cover is from the article published in Journal of Modern Physics, 2014, Vol. 5, No. 4, pp. 137-144 by Mirzoaziz A. Khusenov, *et al.* 

OPEN ACCESS JMP

# Journal of Modern Physics (JMP)

## **Journal Information**

#### SUBSCRIPTIONS

The *Journal of Modern Physics* (Online at Scientific Research Publishing, <a href="www.SciRP.org">www.SciRP.org</a>) is published monthly by Scientific Research Publishing, Inc., USA.

# **Subscription rates:**

Print: \$89 per issue.

To subscribe, please contact Journals Subscriptions Department, E-mail: <a href="mailto:sub@scirp.org">sub@scirp.org</a>

#### **SERVICES**

#### Advertisements

Advertisement Sales Department, E-mail: <a href="mailto:service@scirp.org">service@scirp.org</a>

## Reprints (minimum quantity 100 copies)

Reprints Co-ordinator, Scientific Research Publishing, Inc., USA.

E-mail: sub@scirp.org

# **COPYRIGHT**

#### COPYRIGHT AND REUSE RIGHTS FOR THE FRONT MATTER OF THE JOURNAL:

Copyright © 2014 by Scientific Research Publishing Inc.

This work is licensed under the Creative Commons Attribution International License (CC BY). http://creativecommons.org/licenses/by/4.0/

# COPYRIGHT FOR INDIVIDUAL PAPERS OF THE JOURNAL:

Copyright  $\ensuremath{\mathbb{Q}}$  2014 by author(s) and Scientific Research Publishing Inc.

# REUSE RIGHTS FOR INDIVIDUAL PAPERS:

Note: At SCIRP authors can choose between CC BY and CC BY-NC. Please consult each paper for its reuse rights.

## DISCLAIMER OF LIABILITY

Statements and opinions expressed in the articles and communications are those of the individual contributors and not the statements and opinion of Scientific Research Publishing, Inc. We assume no responsibility or liability for any damage or injury to persons or property arising out of the use of any materials, instructions, methods or ideas contained herein. We expressly disclaim any implied warranties of merchantability or fitness for a particular purpose. If expert assistance is required, the services of a competent professional person should be sought.

# PRODUCTION INFORMATION

For manuscripts that have been accepted for publication, please contact:

E-mail: jmp@scirp.org