ISSN: 2332-5968 Volume 11, Number 3, July 2023

Scientific Research Publishing

Computational Chemistry

ISSN: 2332-5968

https://www.scirp.org/journal/cc

Journal Editorial Board

ISSN 2332-5968 (Print) ISSN 2332-5984 (Online)

https://www.scirp.org/journal/cc

Editor-in-Chief

Prof. Anwar El-Shahawy Assiut University, Egypt

Editorial Board

Dr. Ali Khalaf Al-Matar University of Jordan, Jordan
Dr. Enrique Arribas University of Castilla-La Mancha, Spain
Prof. Nagarajan Arumugam PSG College of Pharmacy, India
Dr. Tamafo Fouegue Aymard Didier The University of Bertoua, Cameroon
Prof. Todor Dudev Sofia University, Bulgaria
Dr. Natalja Fjodorova National Institute of Chemistry, Slovenia
Dr. Soumadwip Ghosh La Jolla, USA
Dr. Selcuk Gümüs Yuzuncu Yil University, Turkey
Dr. Weiwei Han Jilin University, China
Prof. Alireza Heidari California South University, USA
Prof. Parasuraman Jaisankar Indian Institute of Chemical Biology, India
Dr. C. Gopi Mohan Amrita Institute of Medical Sciences and Research Center, India
Dr. Floriano Paes Silva Junior Instituto Oswaldo Cruz, Brazil
Dr. Carlos P. Sosa Cray Inc and University of Minnesota, USA
Prof. Hilal S. Wahab Al-Nahrain University, Iraq
Dr. Carline Josette Weinberg Roumanian Academy, Romania
Dr. Julliane Yoneda Universidade Federal Fluminense, Brazil
Prof. Abdelkader Zarrouk Mohammed First University, Morocco

Scientific Research Publishing

Computational Chemistry, 2023, 11, 53-80
https://www.scirp.org/journal/cc
ISSN Online: 2332-5984
ISSN Print: 2332-5968

Table of Contents

Volume 11 Number 3 July 2023

Functionality of Covalent Organic Framework (COF) in Gas Storage Application: First Principal Study

M. Alharbi, R. Aljohani, R. Alzahrani, Y. Alsufyani, N. Alsumani……53

Design of New Thiadiazole Derivatives with Improved Antidiabetic Activity

C. N. D. Dou, G. S. Dembele, M. G.-R. Kone, N. T. Tuo, F. Konate, A. Niare, P. Karamanis, N. Ziao……67

Computational Chemistry (CC)
Journal Information

SUBSCRIPTIONS

The *Computational Chemistry* (Online at Scientific Research Publishing, https://www.scirp.org/) is published quarterly by Scientific Research Publishing, Inc., USA.

Subscription rates:
Print: $39 per issue.
To subscribe, please contact Journals Subscriptions Department, E-mail: sub@scirp.org

SERVICES

Advertisements
Advertisement Sales Department, E-mail: service@scirp.org

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 © 2023 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 © 2023 by author(s) and Scientific Research Publishing Inc.

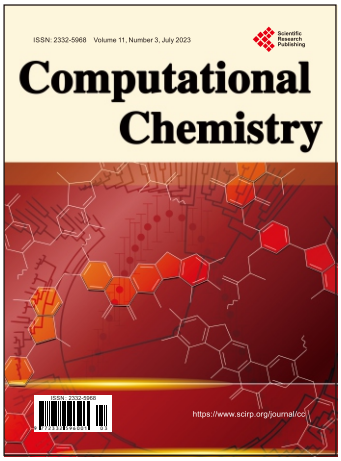
Reuse rights for individual papers:
Note: At SCIRP authors can choose between CC BY and CC BY-NC. Please consult each paper for its reuse rights.

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: cc@scirp.org

Call for Papers



Computational Chemistry

ISSN: 2332-5968 (Print), 2332-5984 (Online)
https://www.scirp.org/journal/cc

Editorial Board

Dr. Ali Khalaf Al-Matar
Dr. Enrique Arribas
Prof. Nagarajan Arumugam
Dr. Tamafo Fouegue Aymard Didier
Prof. Todor Dudev
Dr. Natalja Fjodorova
Dr. Soumadwip Ghosh
Dr. Selcuk Gümüs
Dr. Weiwei Han
Prof. Alireza Heidari
Prof. Parasuraman Jaisankar
Dr. C. Gopi Mohan
Dr. Floriano Paes Silva Junior
Dr. Carlos P. Sosa
Prof. Hilal S. Wahab
Dr. Carline Josette Weinberg
Dr. Julliane Yoneda
Prof. Abdelkader Zarrouk

Subject Coverage

Computational Chemistry (CC) is a unique platform for publishing novel ideas, research outcomes and fundamental advances in all aspects of computational chemistry. All manuscripts must be prepared in English, and are subject to a rigorous and fair peer-review process. The journal publishes original papers including but not limited to the following fields:

- *Ab Initio* Quantum Mechanics
- Chemical Artificial Intelligence
- Chemical Computer-Assisted Instruction
- Cheminformatics
- Chemistry Database
- Code Benchmarking
- Computational Analytical Chemistry
- Computational Biochemistry
- Computational Biophysics
- Computational Colloidal Chemistry
- Computational Electro-Chemistry
- Computational Nanochemistry
- Computational Surface Chemistry
- Computer Molecular Modeling
- Computer-Aided Drug Design
- Data Acquisition, Statistic Analysis and Other Applications
- Density Functional Theory
- Force Field Development and Testing
- Molecular Design
- Molecular Dynamics
- Molecular Mechanics
- Molecular Modeling
- Molecular Simulation
- Molecular Structure Modeling and Image Display
- Quantum Chemistry Calculation
- Semi-Empirical Quantum Mechanics
- Statistical Mechanics
- Theoretical Inorganic Chemistry
- Theoretical Organic Chemistry
- Theoretical Thermo Chemistry

We are also interested in: 1) Short reports—2-5 page papers where an author can present an idea with theoretical background, but has not yet completed the research needed for a complete paper or an author presents preliminary data; 2) Short communications—2-5 page papers; 3) Technical notes—2-5 page papers; 4) Letters to the Editor (the number of pages is not restricted); 5) Reviews or book reviews—comments and critiques (the number of pages is not restricted); 6) Advertisement – 1-2 page papers; 7) News Letters – 1-5 page papers.

Website and E-Mail

https://www.scirp.org/journal/cc **E-mail: cc@scirp.org**