

ISSN: 2332-5968 Volume 9, Number 1, January 2021



# Computational Chemistry



ISSN: 2332-5968



9 772332 596001 01

<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

**Prof. Todor Dudev**

Sofia University, Bulgaria

**Dr. Natalja Fjodorova**

National Institute of Chemistry, Slovenia

**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

# Table of Contents

**Volume 9    Number 1**

**January 2021**

## **DFT Study of Dimerization Sites in Imidazo[1,2-a]pyridinyl-chalcone Series**

B. Konate, S. T. Affi, N. Ziao.....1

## **Computational Stimulation and Experimental Study on Corrosion Inhibition Qualities of *Emilia sonchifolia* Leaf Extract for Copper (CU131729) in Hydrochloric Acid**

R. S. Oguike, O. Oni, A. U. Barambu, D. Balarak, T. Buba, C. U. Okeke, L. S. Momoh, S. Onimisi, W. J. Nwada...18

## **Corrosion Inhibition of Aluminium in Gas and Acid Media by Some Chalcone-Based N-(3-Aminopropyl)Imidazoles: TD-DFT-Based FMO, Conceptual DFT, QTAIM and EDA Studies**

F. K. Bine, S. N. Tasheh, N. K. Nkungli, J. N. Ghogomu.....37

## **Theoretical Studies of Photodynamic Therapy Properties of Azopyridine $\delta$ -OsCl<sub>2</sub>(Azpy)<sub>2</sub> Complex as a Photosensitizer by a TDDFT Method**

W. P. Ouattara, K. Bamba, A. S. Thomas, F. Diarrassouba, L. Ouattara, M. P. Ouattara, K. N. N'guessan,  
M. G. R. Kone, C. G. Kodjo, N. Ziao.....64

## **Hydrogen Bonds Sites of Amylose or Amylopectin from Starch at the ONION Level (B3LYP/6-311++G [d, p]: AM1)**

A. A. Valentin, N. B. Robert, B. El H. Sawaliho.....85

## 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](mailto:sub@scirp.org)

#### SERVICES

##### **Advertisements**

Advertisement Sales Department, E-mail: [service@scirp.org](mailto:service@scirp.org)

##### **Reprints (minimum quantity 100 copies)**

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

E-mail: [sub@scirp.org](mailto:sub@scirp.org)

#### COPYRIGHT

##### **Copyright and reuse rights for the front matter of the journal:**

Copyright © 2021 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 © 2021 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.

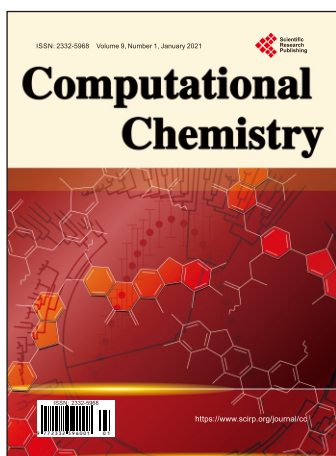
##### **Disclaimer of liability**

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](mailto:cc@scirp.org)



# 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

Prof. Todor Dudev

Dr. Natalja Fjodorova

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](mailto:cc@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 with its publication.

## *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, worldwide, 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: <https://www.scirp.org>**  
**Subscription: [sub@scirp.org](mailto:sub@scirp.org)**  
**Advertisement: [service@scirp.org](mailto:service@scirp.org)**