Green Journals

International Approved Journals

Journal Information

Journal Title	JOURNAL OF COMPUTATIONAL CHEMISTRY
Publisher	WILEY
ISSN	0192-8651
E-ISSN	1096-987X
Database	Clarivate
Domain	Life Sciences, Physical Sciences, Social Sciences

Classification History

Year	A+	A	B	C
2026		✓	✓	
2025		✓	✓	
2024		✓	✓	
2023		✓	✓	
2021/2022		✓	✓	
2020		✓	✓	
2019		✓	✓	
2018		✓		

Classification: The table above shows all journal classifications recorded for each classification year in the Green Journals database. A journal may have more than one classification in the same year.

Recent Articles

Issue Information
2026-11-6 Vol. 47 Issue 30
DOI: 10.1002/jcc.70428

<scp>Sc</scp> ₂ @ <scp> C ₆₆ </scp> . Spherical Aromaticity in a Markedly Ellipsoidal Endohedral Metallic Fullerene
2026-11-6 Vol. 47 Issue 30
Authors: Desmond Macleod-Carey, Alvaro Muñoz-Castro
DOI: 10.1002/jcc.70531

Carbyne-Terminated Carbon-Flanked Noble-Gas Cations: Stability and Asymmetric C–Ng–C Bonding (Ng He–Rn)
2026-11-6 Vol. 47 Issue 30
Authors: Leonardo S. Reyes-Fernández, Esteban Flores-Gutiérrez, Esteban Marambio et al.
DOI: 10.1002/jcc.70546

<scp>LTVAE</scp> : Hybrid <scp>LSTM</scp> -Transformer <scp>VAE</scp> Architecture for Molecular <scp>SMILES</scp> Representation
2026-11-3 Vol. 47 Issue 29
Authors: Md Halim Mondol, Qingshan Wei, Edgar Lobaton
DOI: 10.1002/jcc.70521

Theoretical Investigation of Ethane-to-Aromatics Conversion Over [<scp> GaH ₂ </scp>]- <scp>ZSM</scp> -5
2026-11-3 Vol. 47 Issue 29
Authors: João V. F. Costa, Thiago M. Mizumoto, Lenin J. Díaz Soto et al.
DOI: 10.1002/jcc.70537

Issue Information
2026-11-2 Vol. 47 Issue 29
DOI: 10.1002/jcc.70427

Physics-Based <scp>AI</scp> -Augmented Workflows Discovering Candidate Graphene Quantum Dot Near-Infrared Chromophores
2026-11-2 Vol. 47 Issue 29
Authors: Naga Mani Gajula, Muhammad Hammad Ali, Md. Masud Rana et al.
DOI: 10.1002/jcc.70522

Reduced-Dimensional Reaction-Space Analysis of a Trispericyclic Reaction by <scp>ReSPer</scp>
2026-11-2 Vol. 47 Issue 29
Authors: Takuro Tsutsumi, Akifumi Fujita, Yuriko Ono et al.
DOI: 10.1002/jcc.70539

Relativistic Effects on Bond Critical Points and Basin Population on Heavy-Atom-Containing Molecules With the Modified Dirac Equation
2026-10-28 Vol. 47 Issue 28
Authors: Andy D. Zapata-Escobar, Alejandro F. Maldonado
DOI: 10.1002/jcc.70538

Assessing Structural, Thermal, and Mechanical Properties of Zirconium-Based Metal-Organic Frameworks via <scp>DFTB3</scp> / <scp>3OB MD</scp> Simulations: A Benchmark Beyond <scp>UiO</scp> Frameworks
2026-10-28 Vol. 47 Issue 28
Authors: Armin Penz, Thomas S. Hofer
DOI: 10.1002/jcc.70536