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Journal Information

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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

A Quantum-HPC Hybrid Workflow for Reaction-Center Electronic Dynamics: Application to a Cytochrome P450-Inspired Iron-Complex Model
2026-10-31
Authors: Shintaro Maekawa, Takao Otsuka, Riku Masui et al.
DOI: 10.1021/acs.jctc.6c01410

A Machine-Learned Symbolic Committor for a Chemical Reaction: Isomerization in Retinal and p -Coumaric Acid
2026-10-30
Authors: Kai Töpfer, Gianmarco Lazzeri, Vittoria Ossanna et al.
DOI: 10.1021/acs.jctc.6c01496

Global Potential Energy Surface Exploration Using Generative Stochastic Surface Walking (Gen-SSW)
2026-10-30
Authors: Qiming Liang, Zi-Xing Guo, Jin-Peng Tang et al.
DOI: 10.1021/acs.jctc.6c01420

Correction to “Thermodynamic Perturbation Theory for Charged Branched Polymers”
2026-10-30
Authors: Leying Qing, Xiujun Wang, Shichao Li et al.
DOI: 10.1021/acs.jctc.6c02133

An Efficient Neural Network Architecture for Molecular Vibrational States: From Rigid Molecules to Molecular Complexes
2026-10-30
Authors: Shuaishuai Zhao, Dong H. Zhang
DOI: 10.1021/acs.jctc.6c01254

Algorithm for Locating SCF Solutions Reveals Conceptual Limitations of the Broken-Symmetry Approach Applied to the Oxygen-Evolving Complex
2026-10-30
Authors: Pavel Pokhilko, Yulia Pushkar
DOI: 10.1021/acs.jctc.6c01499

Data-Driven Approach for Predicting Long-Time Anomalous Transport from Short Trajectories
2026-10-29
Authors: Chuyi Liu, Yifeng Guan, Jingyuan Li et al.
DOI: 10.1021/acs.jctc.6c01846

Paired-Isotopologue Hessian Benchmarking for Second-Order Validation of Machine-Learned Water Potentials
2026-10-29
Authors: Yihao Wen, Xue Wen, Baoxin Ni et al.
DOI: 10.1021/acs.jctc.6c01692

Unraveling the Ultrafast Photodynamics of Molecular Photoswitches in β-Adrenergic Receptors by First-Principles Nonadiabatic Dynamics Simulations
2026-10-29
Authors: Mohammad Khavani, Amirhossein Bakhtiiari, Ruibin Liang
DOI: 10.1021/acs.jctc.6c01210

Multistate-Averaged Kohn–Sham ΔSCF Method for Excitation Energies, Transition Properties, and Absorption Spectra and Its Relation to Ensemble Density Functional Theory
2026-10-28
Authors: Oliver Bertleff, Egor Trushin, Andreas Görling
DOI: 10.1021/acs.jctc.6c01397