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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		✓		

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Recent Articles

Real-space vs interelectronic exchange mixing for the prediction of low-lying Rydberg excitations within time-dependent density functional theory
2026-10-28 Vol. 165 Issue 16
Authors: Tiffany T. Nguyen, Jacob A. Que, Robin Grotjahn
DOI: 10.1063/5.0356718

Third-order size-consistent Brillouin-Wigner perturbation theory
2026-10-28 Vol. 165 Issue 16
Authors: Zhenling Wang, Martin Head-Gordon
DOI: 10.1063/5.0352348

Position-and conformation-dependent effects of fluorination on the structure and methyl internal rotation of methyl benzoates
2026-10-28 Vol. 165 Issue 16
Authors: Xiujuan Wang, Philipp Buschmann, Wenqi Lv et al.
DOI: 10.1063/5.0356016

Chiral vibrational modes and vibrational circular dichroism
2026-10-28 Vol. 165 Issue 16
Authors: Xuecheng Tao, Clàudia Climent, Ethan Abraham et al.
DOI: 10.1063/5.0353819

Origin of long-lived nuclear spin states and coherences in aliphatic chains revealed by relaxation theory
2026-10-28 Vol. 165 Issue 16
Authors: Danil A. Markelov, Kirill F. Sheberstov
DOI: 10.1063/5.0355673

Symmetry adapted auxiliary density perturbation theory

2026-10-28 Vol. 165 Issue 16
Authors: José A. Flores-Ramos, Roberto Flores-Moreno
DOI: 10.1063/5.0347044

Nonlinear canonical transformations for studying spin-1/2 Hamiltonians

2026-10-28 Vol. 165 Issue 16
Authors: Swarnamoy Ghosh, Thomas M. Henderson, Gustavo E. Scuseria
DOI: 10.1063/5.0355030

Signatures of auxeticity in microgels at low and ultralow crosslinker concentration

2026-10-28 Vol. 165 Issue 16
Authors: Susana Marín-Aguilar, Leah Rank, Emanuela Zaccarelli
DOI: 10.1063/5.0355700

Recent developments in TURBOMOLE

2026-10-28 Vol. 165 Issue 16
Authors: Yannick J. Franzke, Manas Sharma, Priyanshi Bhasin et al.
DOI: 10.1063/5.0351594

Hybrid mechanics of coupled qubits

2026-10-28 Vol. 165 Issue 16
Authors: Merfat Alzomai, Dmitrii V. Shalashilin
DOI: 10.1063/5.0349433