

# Combining Machine Learning and Computational Chemistry in Chemical Systems

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Higher-Order Explanations of Graph Neural Networks via Relevant Walks. IEEE Transactions on Pattern Analysis and Machine Intelligence, 2022, 44, 7581-7596.	13.9	58
2	Topological Characterization and Graph Entropies of Tessellations of Kekulene Structures: Existence of Isentropic Structures and Applications to Thermochemistry, Nuclear Magnetic Resonance, and Electron Spin Resonance. Journal of Physical Chemistry A, 2021, 125, 8140-8158.	2.5	46
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16	Dimensionality reduction in machine learning for nonadiabatic molecular dynamics: Effectiveness of elemental sublattices in lead halide perovskites. Journal of Chemical Physics, 2022, 156, 054110.	3.0	4
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18	A Concise Review on Recent Developments of Machine Learning for the Prediction of Vibrational Spectra. Journal of Physical Chemistry A, 2022, 126, 801-812.	2.5	19

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