## **Eleftherios Lambros**

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. Nature Communications, 2021, 12, 6359.	12.8	45
2	How good are polarizable and flexible models for water: Insights from a many-body perspective. Journal of Chemical Physics, 2020, 153, 060901.	3.0	39
3	Low-order many-body interactions determine the local structure of liquid water. Chemical Science, 2019, 10, 8211-8218.	7.4	35
4	General Many-Body Framework for Data-Driven Potentials with Arbitrary Quantum Mechanical Accuracy: Water as a Case Study. Journal of Chemical Theory and Computation, 2021, 17, 5635-5650.	5.3	28
5	Anomalies and Local Structure of Liquid Water from Boiling to the Supercooled Regime as Predicted by the Many-Body MB-pol Model. Journal of Physical Chemistry Letters, 2022, 13, 3652-3658.	4.6	25
6	Modeling Membrane Protein–Ligand Binding Interactions: The Human Purinergic Platelet Receptor. Journal of Physical Chemistry B, 2016, 120, 12293-12304.	2.6	24
7	Assessing the Interplay between Functional-Driven and Density-Driven Errors in DFT Models of Water. Journal of Chemical Theory and Computation, 2022, 18, 3410-3426.	5.3	14
8	Highly Accurate Many-Body Potentials for Simulations of N <sub>2</sub> O <sub>5</sub> in Water: Benchmarks, Development, and Validation. Journal of Chemical Theory and Computation, 2021, 17, 3931-3945.	5.3	13
9	Assessing the Accuracy of the SCAN Functional for Water through a Many-Body Analysis of the Adiabatic Connection Formula. Journal of Chemical Theory and Computation, 2021, 17, 3739-3749.	5.3	13
10	A Many-Body, Fully Polarizable Approach to QM/MM Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7462-7472.	5.3	11
11	Density functional theory of water with the machine-learned DM21 functional. Journal of Chemical Physics, 2022, 156, 161103.	3.0	8