Pablo M Piaggi

List of Publications by Year
in descending order

21 papers	790 citations	567281 15 h-index	713466 21 g-index
22 all docs	22 docs citations	22 times ranked	754 citing authors

#	Article	IF	Citations
1	Phase diagram of the TIP4P/Ice water model by enhanced sampling simulations. Journal of Chemical Physics, 2022, 157, .	3.0	8
2	Enhancing the formation of ionic defects to study the ice Ih/XI transition with molecular dynamics simulations. Molecular Physics, 2021, 119, .	1.7	7
3	Phase Equilibrium of Water with Hexagonal and Cubic Ice Using the SCAN Functional. Journal of Chemical Theory and Computation, 2021, 17, 3065-3077.	5.3	37
4	A Computational Study of RNA Tetraloop Thermodynamics, Including Misfolded States. Journal of Physical Chemistry B, 2021, 125, 13685-13695.	2.6	5
5	Signatures of a liquidâ€“liquid transition in an ab initio deep neural network model for water. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 26040-26046.	7.1	112
6	Unified Approach to Enhanced Sampling. Physical Review X, 2020, 10, .	8.9	43
7	Phase equilibrium of liquid water and hexagonal ice from enhanced sampling molecular dynamics simulations. Journal of Chemical Physics, 2020, 152, 204116.	3.0	15
8	Ab initio phase diagram and nucleation of gallium. Nature Communications, 2020, 11, 2654.	12.8	102
9	Calculation of phase diagrams in the multithermal-multibaric ensemble. Journal of Chemical Physics, 2019, 150, 244119.	3.0	29
10	Molecular Dynamics Simulations of Crystal Nucleation from Solution at Constant Chemical Potential. Journal of Chemical Theory and Computation, 2019, 15, 6923-6930.	5.3	31
11	A local fingerprint for hydrophobicity and hydrophilicity: From methane to peptides. Journal of Chemical Physics, 2019, 150, 204103.	3.0	4
12	Naphthalene crystal shape prediction from molecular dynamics simulations. CrystEngComm, 2019, 21, 3280-3288.	2.6	19
13	Multithermal-Multibaric Molecular Simulations from a Variational Principle. Physical Review Letters, 2019, 122, 050601.	7.8	22
14	A Cannibalistic Approach to Grand Canonical Crystal Growth. Journal of Chemical Theory and Computation, 2018, 14, 2678-2683.	5.3	18
15	Searching for Entropically Stabilized Phases: The Case of Silver Iodide. Journal of Physical Chemistry C, 2018, 122, 1786-1790.	3.1	18
16	Predicting polymorphism in molecular crystals using orientational entropy. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10251-10256.	7.1	57
17	Molecular dynamics simulations of liquid silica crystallization. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 5348-5352.	7.1	78
18	Entropy based fingerprint for local crystalline order. Journal of Chemical Physics, 2017, 147, 114112.	3.0	92

#	Article	IF	Citations
19	Enhancing Entropy and Enthalpy Fluctuations to Drive Crystallization in Atomistic Simulations. Physical Review Letters, 2017, 119, 015701.	7.8	74
20	A variational approach to nucleation simulation. Faraday Discussions, 2016, 195, 557-568.	3.2	15
21	Application to large systems: general discussion. Faraday Discussions, 2016, 195, 671-698.	3.2	4