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	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
2	Ab initio phase diagram and nucleation of gallium. Nature Communications, 2020, 11, 2654.	12.8	102
3	Entropy based fingerprint for local crystalline order. Journal of Chemical Physics, 2017, 147, 114112.	3.0	92
4	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
5	Enhancing Entropy and Enthalpy Fluctuations to Drive Crystallization in Atomistic Simulations. Physical Review Letters, 2017, 119, 015701.	7.8	74
6	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
7	Unified Approach to Enhanced Sampling. Physical Review X, 2020, 10, .	8.9	43
8	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
9	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
10	Calculation of phase diagrams in the multithermal-multibaric ensemble. Journal of Chemical Physics, 2019, 150, 244119.	3.0	29
11	Multithermal-Multibaric Molecular Simulations from a Variational Principle. Physical Review Letters, 2019, 122, 050601.	7.8	22
12	Naphthalene crystal shape prediction from molecular dynamics simulations. CrystEngComm, 2019, 21, 3280-3288.	2.6	19
13	A Cannibalistic Approach to Grand Canonical Crystal Growth. Journal of Chemical Theory and Computation, 2018, 14, 2678-2683.	5.3	18
14	Searching for Entropically Stabilized Phases: The Case of Silver Iodide. Journal of Physical Chemistry C, 2018, 122, 1786-1790.	3.1	18
15	A variational approach to nucleation simulation. Faraday Discussions, 2016, 195, 557-568.	3.2	15
16	Phase equilibrium of liquid water and hexagonal ice from enhanced sampling molecular dynamics simulations. Journal of Chemical Physics, 2020, 152, 204116.	3.0	15
17	Phase diagram of the TIP4P/Ice water model by enhanced sampling simulations. Journal of Chemical Physics, 2022, 157, .	3.0	8
18	Enhancing the formation of ionic defects to study the ice Ih/XI transition with molecular dynamics simulations. Molecular Physics, 2021, 119, .	1.7	7

#	Article	IF	Citations
19	A Computational Study of RNA Tetraloop Thermodynamics, Including Misfolded States. Journal of Physical Chemistry B, 2021, 125, 13685-13695.	2.6	5
20	Application to large systems: general discussion. Faraday Discussions, 2016, 195, 671-698.	3.2	4
21	A local fingerprint for hydrophobicity and hydrophilicity: From methane to peptides. Journal of Chemical Physics, 2019, 150, 204103.	3.0	4