Alex Rodriguez

List of Publications by Year
in descending order

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15 papers	4,289 citations	687363 13 h-index	996975 15 g-index
15 all docs	15 docs citations	15 times ranked	5013 citing authors

#	Article	IF	Citations
1	High-Dimensional Fluctuations in Liquid Water: Combining Chemical Intuition with Unsupervised Learning. Journal of Chemical Theory and Computation, 2022, 18, 3136-3150.	5.3	14
2	Candidate Binding Sites for Allosteric Inhibition of the SARS-CoV-2 Main Protease from the Analysis of Large-Scale Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2021, 12, 65-72.	4.6	18
3	Unsupervised Learning Universal Critical Behavior via the Intrinsic Dimension. Physical Review X, 2021, 11, .	8.9	26
4	Unsupervised Learning Methods for Molecular Simulation Data. Chemical Reviews, 2021, 121, 9722-9758.	47.7	182
5	Automatic topography of high-dimensional data sets by non-parametric density peak clustering. Information Sciences, 2021, 560, 476-492.	6.9	25
6	Intrinsic Dimension of Path Integrals: Data-Mining Quantum Criticality and Emergent Simplicity. PRX Quantum, 2021, 2, .	9.2	18
7	Explicit Characterization of the Free-Energy Landscape of a Protein in the Space of All Its C_{Î±} Carbons. Journal of Chemical Theory and Computation, 2020, 16, 80-87.	5.3	15
8	The mechanism of RNA base fraying: Molecular dynamics simulations analyzed with core-set Markov state models. Journal of Chemical Physics, 2019, 150, 154123.	3.0	24
9	Computing the Free Energy without Collective Variables. Journal of Chemical Theory and Computation, 2018, 14, 1206-1215.	5.3	37
10	The permeation mechanism of organic cations through a CNG mimic channel. PLoS Computational Biology, 2018, 14, e1006295.	3.2	1
11	METAGUI 3: A graphical user interface for choosing the collective variables in molecular dynamics simulations. Computer Physics Communications, 2017, 217, 204-209.	7.5	34
12	Estimating the intrinsic dimension of datasets by a minimal neighborhood information. Scientific Reports, 2017, 7, 12140.	3.3	135
13	A structural, functional, and computational analysis suggests pore flexibility as the base for the poor selectivity of CNG channels. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E3619-28.	7.1	35
14	Clustering by fast search and find of density peaks. Science, 2014, 344, 1492-1496.	12.6	3,709
15	Computational Study of the Free Energy Landscape of the Miniprotein CLN025 in Explicit and Implicit Solvent. Journal of Physical Chemistry B, 2011, 115, 1440-1449.	2.6	16