Omar Valsson

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1423478/publications.pdf

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32	1,692	430442	454577
papers	citations	18 h-index	30 g-index

34	34	34	1771
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Enhancing Important Fluctuations: Rare Events and Metadynamics from a Conceptual Viewpoint. Annual Review of Physical Chemistry, 2016, 67, 159-184.	4.8	497
2	Variational Approach to Enhanced Sampling and Free Energy Calculations. Physical Review Letters, 2014, 113, 090601.	2.9	206
3	Photoisomerization of Model Retinal Chromophores: Insight from Quantum Monte Carlo and Multiconfigurational Perturbation Theory. Journal of Chemical Theory and Computation, 2010, 6, 1275-1292.	2.3	126
4	Electronic Excitations of Simple Cyanine Dyes: Reconciling Density Functional and Wave Function Methods. Journal of Chemical Theory and Computation, 2011, 7, 444-455.	2.3	124
5	Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls. Journal of Chemical Theory and Computation, 2013, 9, 2441-2454.	2.3	81
6	Enhancing Entropy and Enthalpy Fluctuations to Drive Crystallization in Atomistic Simulations. Physical Review Letters, 2017, 119, 015701.	2.9	74
7	State-Specific Embedding Potentials for Excitation-Energy Calculations. Journal of Chemical Theory and Computation, 2013, 9, 2355-2367.	2.3	70
8	Frequency adaptive metadynamics for the calculation of rare-event kinetics. Journal of Chemical Physics, 2018, 149, 072309.	1.2	54
9	Excitation energies of retinal chromophores: critical role of the structural model. Physical Chemistry Chemical Physics, 2012, 14, 11015.	1.3	48
10	Enhanced, targeted sampling of high-dimensional free-energy landscapes using variationally enhanced sampling, with an application to chignolin. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1150-1155.	3.3	47
11	Well-Tempered Variational Approach to Enhanced Sampling. Journal of Chemical Theory and Computation, 2015, 11, 1996-2002.	2.3	42
12	Variationally Optimized Free-Energy Flooding for Rate Calculation. Physical Review Letters, 2015, 115, 070601.	2.9	35
13	Coarse graining from variationally enhanced sampling applied to the Ginzburgâ€“Landau model. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3370-3374.	3.3	35
14	Finding multiple reaction pathways of ligand unbinding. Journal of Chemical Physics, 2019, 150, 221101.	1.2	30
15	Electrostatic versus Resonance Interactions in Photoreceptor Proteins: The Case of Rhodopsin. Journal of Physical Chemistry Letters, 2016, 7, 4547-4553.	2.1	25
16	Variational Flooding Study of a S_N2 Reaction. Journal of Physical Chemistry Letters, 2017, 8, 580-583.	2.1	23
17	Multiscale Reweighted Stochastic Embedding: Deep Learning of Collective Variables for Enhanced Sampling. Journal of Physical Chemistry A, 2021, 125, 6286-6302.	1.1	22
18	Gas-Phase Retinal Spectroscopy: Temperature Effects Are But a Mirage. Journal of Physical Chemistry Letters, 2012, 3, 908-912.	2.1	19

#	Article	IF	Citations
19	Thermodynamical Description of a Quasi-First-Order Phase Transition from the Well-Tempered Ensemble. Journal of Chemical Theory and Computation, 2013, 9, 5267-5276.	2.3	16
20	Conformational Entropy as Collective Variable for Proteins. Journal of Physical Chemistry Letters, 2017, 8, 4752-4756.	2.1	16
21	Regarding the use and misuse of retinal protonated Schiff base photochemistry as a test case for time-dependent density-functional theory. Journal of Chemical Physics, 2015, 142, 144104.	1.2	15
22	A variational approach to nucleation simulation. Faraday Discussions, 2016, 195, 557-568.	1.6	15
23	Coherent switching by detuning a side-coupled quantum-dot system. Physical Review B, 2008, 78, .	1.1	11
24	Bespoke Bias for Obtaining Free Energy Differences within Variationally Enhanced Sampling. Journal of Chemical Theory and Computation, 2016, 12, 2162-2169.	2.3	11
25	Acrylic Paints: An Atomistic View of Polymer Structure and Effects of Environmental Pollutants. Journal of Physical Chemistry B, 2021, 125, 10854-10865.	1.2	11
26	Mg²⁺ Sensing by an RNA Fragment: Role of Mg²⁺-Coordinated Water Molecules. Journal of Chemical Theory and Computation, 2020, 16, 6702-6715.	2.3	9
27	Free-energy landscape of polymer-crystal polymorphism. Soft Matter, 2020, 16, 9683-9692.	1.2	9
28	Chemical potential calculations in non-homogeneous liquids. Journal of Chemical Physics, 2018, 149, 072305.	1.2	8
29	Hierarchical Protein Free Energy Landscapes from Variationally Enhanced Sampling. Journal of Chemical Theory and Computation, 2016, 12, 5751-5757.	2.3	5
30	Variationally Enhanced Sampling. , 2020, , 621-634.		4
31	Improving the Efficiency of Variationally Enhanced Sampling with Wavelet-Based Bias Potentials. Journal of Chemical Theory and Computation, 2022, 18, 4127-4141.	2.3	3
32	Variationally Enhanced Sampling. , 2018, , 1-14.		1