Omar Valsson

List of Publications by Year
in descending order

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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	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
2	Multiscale Reweighted Stochastic Embedding: Deep Learning of Collective Variables for Enhanced Sampling. Journal of Physical Chemistry A, 2021, 125, 6286-6302.	1.1	22
3	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
4	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
5	Free-energy landscape of polymer-crystal polymorphism. Soft Matter, 2020, 16, 9683-9692.	1.2	9
6	Variationally Enhanced Sampling. , 2020, , 621-634.		4
7	Finding multiple reaction pathways of ligand unbinding. Journal of Chemical Physics, 2019, 150, 221101.	1.2	30
8	Variationally Enhanced Sampling. , 2018, , 1-14.		1
9	Chemical potential calculations in non-homogeneous liquids. Journal of Chemical Physics, 2018, 149, 072305.	1.2	8
10	Frequency adaptive metadynamics for the calculation of rare-event kinetics. Journal of Chemical Physics, 2018, 149, 072309.	1.2	54
11	Variational Flooding Study of a S_N2 Reaction. Journal of Physical Chemistry Letters, 2017, 8, 580-583.	2.1	23
12	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
13	Conformational Entropy as Collective Variable for Proteins. Journal of Physical Chemistry Letters, 2017, 8, 4752-4756.	2.1	16
14	Enhancing Entropy and Enthalpy Fluctuations to Drive Crystallization in Atomistic Simulations. Physical Review Letters, 2017, 119, 015701.	2.9	74
15	A variational approach to nucleation simulation. Faraday Discussions, 2016, 195, 557-568.	1.6	15
16	Bespoke Bias for Obtaining Free Energy Differences within Variationally Enhanced Sampling. Journal of Chemical Theory and Computation, 2016, 12, 2162-2169.	2.3	11
17	Electrostatic versus Resonance Interactions in Photoreceptor Proteins: The Case of Rhodopsin. Journal of Physical Chemistry Letters, 2016, 7, 4547-4553.	2.1	25
18	Hierarchical Protein Free Energy Landscapes from Variationally Enhanced Sampling. Journal of Chemical Theory and Computation, 2016, 12, 5751-5757.	2.3	5

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19	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
20	Enhancing Important Fluctuations: Rare Events and Metadynamics from a Conceptual Viewpoint. Annual Review of Physical Chemistry, 2016, 67, 159-184.	4.8	497
21	Variationally Optimized Free-Energy Flooding for Rate Calculation. Physical Review Letters, 2015, 115, 070601.	2.9	35
22	Well-Tempered Variational Approach to Enhanced Sampling. Journal of Chemical Theory and Computation, 2015, 11, 1996-2002.	2.3	42
23	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
24	Variational Approach to Enhanced Sampling and Free Energy Calculations. Physical Review Letters, 2014, 113, 090601.	2.9	206
25	Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls. Journal of Chemical Theory and Computation, 2013, 9, 2441-2454.	2.3	81
26	State-Specific Embedding Potentials for Excitation-Energy Calculations. Journal of Chemical Theory and Computation, 2013, 9, 2355-2367.	2.3	70
27	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
28	Excitation energies of retinal chromophores: critical role of the structural model. Physical Chemistry Chemical Physics, 2012, 14, 11015.	1.3	48
29	Gas-Phase Retinal Spectroscopy: Temperature Effects Are But a Mirage. Journal of Physical Chemistry Letters, 2012, 3, 908-912.	2.1	19
30	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
31	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
32	Coherent switching by detuning a side-coupled quantum-dot system. Physical Review B, 2008, 78, .	1.1	11