Paolo Nicolini

List of Publications by Year
in descending order

25	857	623734 14	580821 25
papers	citations	h-index	g-index

25	25	25	911
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Modeling and simulation in tribology across scales: An overview. Tribology International, 2018, 125, 169-199.	5.9	335
2	Ultra-low friction and edge-pinning effect in large-lattice-mismatch van der Waals heterostructures. Nature Materials, 2022, 21, 47-53.	27.5	110
3	Toward quantitative estimates of binding affinities for proteinâ€“ligand systems involving large inhibitor compounds: A steered molecular dynamics simulation route. Journal of Computational Chemistry, 2013, 34, 1561-1576.	3.3	41
4	A comparison of empirical potentials for sliding simulations of MoS2. Computational Materials Science, 2016, 115, 158-169.	3.0	38
5	Nanoscale frictional properties of ordered and disordered MoS2. Tribology International, 2019, 136, 67-74.	5.9	37
6	Structural Ordering of Molybdenum Disulfide Studied via Reactive Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2018, 10, 8937-8946.	8.0	34
7	On the lubricity of transition metal dichalcogenides: an ab initio study. Nanoscale, 2017, 9, 5597-5607.	5.6	32
8	Exploiting Configurational Freezing in Nonequilibrium Monte Carlo Simulations. Journal of Chemical Theory and Computation, 2011, 7, 582-593.	5.3	29
9	Superlubricity achieved for commensurate sliding: MoS2 frictional anisotropy in silico. Computational Materials Science, 2019, 163, 17-23.	3.0	24
10	Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980.	4.0	23
11	Atomic-scale design of friction and energy dissipation. Physical Review B, 2019, 99, .	3.2	23
12	Hummer and Szabo-like Potential of Mean Force Estimator for Bidirectional Nonequilibrium Pulling Experiments/Simulations. Journal of Physical Chemistry B, 2010, 114, 9546-9554.	2.6	20
13	Improving fast-switching free energy estimates by dynamical freezing. Physical Review E, 2009, 80, 041124.	2.1	17
14	Exploring the Stability of Twisted van der Waals Heterostructures. ACS Applied Materials & Interfaces, 2020, 12, 45214-45221.	8.0	14
15	Features in chemical kinetics. II. A self-emerging definition of slow manifolds. Journal of Chemical Physics, 2013, 138, 234102.	3.0	13
16	Features in chemical kinetics. I. Signatures of self-emerging dimensional reduction from a general format of the evolution law. Journal of Chemical Physics, 2013, 138, 234101.	3.0	10
17	Shortcomings of the standard Lennardâ€“Jones dispersion term in water models, studied with force matching. Journal of Chemical Physics, 2013, 139, 184111.	3.0	10
18	The force matching approach to multiscale simulations: Merits, shortcomings, and future perspectives. International Journal of Quantum Chemistry, 2014, 114, 1036-1040.	2.0	9

#	Article	IF	Citations
19	New Reactive Force Field for Simulations of MoS₂ Crystallization. Journal of Physical Chemistry C, 2022, 126, 9475-9481.	3.1	9
20	Exploring Nanoscale Lubrication Mechanisms of Multilayer MoS2 During Sliding: The Effect of Humidity. Frontiers in Chemistry, 2021, 9, 684441.	3.6	8
21	Features in chemical kinetics. III. Attracting subspaces in a hyper-spherical representation of the reactive system. Journal of Chemical Physics, 2015, 143, 224109.	3.0	6
22	A Low-Computational-Cost Strategy to Localize Points in the Slow Manifold Proximity for Isothermal Chemical Kinetics. International Journal of Chemical Kinetics, 2017, 49, 477-493.	1.6	5
23	Stochastic thermodynamics of nanoscale friction. Physical Review E, 2021, 103, 052104.	2.1	4
24	Attracting subspaces in a hyper-spherical representation of autonomous dynamical systems. Journal of Mathematical Physics, 2017, 58, .	1.1	3
25	Recasting the mass-action rate equations of open chemical reaction networks into a universal quadratic format. Journal of Mathematical Chemistry, 2019, 57, 1001-1018.	1.5	3