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	Ultra-low friction and edge-pinning effect in large-lattice-mismatch van der Waals heterostructures. Nature Materials, 2022, 21, 47-53.	27.5	110
2	New Reactive Force Field for Simulations of MoS₂ Crystallization. Journal of Physical Chemistry C, 2022, 126, 9475-9481.	3.1	9
3	Stochastic thermodynamics of nanoscale friction. Physical Review E, 2021, 103, 052104.	2.1	4
4	Exploring Nanoscale Lubrication Mechanisms of Multilayer MoS2 During Sliding: The Effect of Humidity. Frontiers in Chemistry, 2021, 9, 684441.	3.6	8
5	Exploring the Stability of Twisted van der Waals Heterostructures. ACS Applied Materials & Interfaces, 2020, 12, 45214-45221.	8.0	14
6	Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980.	4.0	23
7	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
8	Superlubricity achieved for commensurate sliding: MoS2 frictional anisotropy in silico. Computational Materials Science, 2019, 163, 17-23.	3.0	24
9	Atomic-scale design of friction and energy dissipation. Physical Review B, 2019, 99, .	3.2	23
10	Nanoscale frictional properties of ordered and disordered MoS2. Tribology International, 2019, 136, 67-74.	5.9	37
11	Structural Ordering of Molybdenum Disulfide Studied via Reactive Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2018, 10, 8937-8946.	8.0	34
12	Modeling and simulation in tribology across scales: An overview. Tribology International, 2018, 125, 169-199.	5.9	335
13	On the lubricity of transition metal dichalcogenides: an ab initio study. Nanoscale, 2017, 9, 5597-5607.	5.6	32
14	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
15	Attracting subspaces in a hyper-spherical representation of autonomous dynamical systems. Journal of Mathematical Physics, 2017, 58, .	1.1	3
16	A comparison of empirical potentials for sliding simulations of MoS2. Computational Materials Science, 2016, 115, 158-169.	3.0	38
17	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
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	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
20	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
21	Features in chemical kinetics. II. A self-emerging definition of slow manifolds. Journal of Chemical Physics, 2013, 138, 234102.	3.0	13
22	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
23	Exploiting Configurational Freezing in Nonequilibrium Monte Carlo Simulations. Journal of Chemical Theory and Computation, 2011, 7, 582-593.	5.3	29
24	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
25	Improving fast-switching free energy estimates by dynamical freezing. Physical Review E, 2009, 80, 041124.	2.1	17