Maxime Vassaux

List of Publications by Year
in descending order

37 papers	1,702 citations	430874 18 h-index	361022 35 g-index
41 all docs	41 docs citations	41 times ranked	2276 citing authors

#	Article	IF	Citations
1	Hybrid parallelization of molecular dynamics simulations to reduce load imbalance. Journal of Supercomputing, 2022, 78, 9184-9215.	3.6	3
2	Large Scale Study of Ligandâ€“Protein Relative Binding Free Energy Calculations: Actionable Predictions from Statistically Robust Protocols. Journal of Chemical Theory and Computation, 2022, 18, 2687-2702.	5.3	14
3	Accelerating Heterogeneous Multiscale Simulations of Advanced Materials Properties with Graphâ€Based Clustering. Advanced Theory and Simulations, 2021, 4, 2000234.	2.8	1
4	VECMAtk: a scalable verification, validation and uncertainty quantification toolkit for scientific simulations. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200221.	3.4	15
5	When we can trust computers (and when we can't). Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200067.	3.4	12
6	Uncertainty quantification in classical molecular dynamics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200082.	3.4	44
7	Ensembles Are Required to Handle Aleatoric and Parametric Uncertainty in Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2021, 17, 5187-5197.	5.3	18
8	Toward High Fidelity Materials Property Prediction from Multiscale Modeling and Simulation. Advanced Theory and Simulations, 2020, 3, 1900122.	2.8	12
9	Actomyosin, vimentin and LINC complex pull on osteosarcoma nuclei to deform on micropillar topography. Biomaterials, 2020, 234, 119746.	11.4	25
10	Building Confidence in Simulation: Applications of EasyVVUQ. Advanced Theory and Simulations, 2020, 3, 1900246.	2.8	21
11	Rapid, accurate, precise and reproducible ligandâ€“protein binding free energy prediction. Interface Focus, 2020, 10, 20200007.	3.0	77
12	From digital hype to analogue reality: Universal simulation beyond the quantum and exascale eras. Journal of Computational Science, 2020, 46, 101093.	2.9	5
13	EasyVVUQ: A Library for Verification, Validation and Uncertainty Quantification in High Performance Computing. Journal of Open Research Software, 2020, 8, 11.	5.9	34
14	Designing Optimal Scaffold Topographies to Promote Nucleus-Guided Mechanosensitive Cell Migration Using in Silico Models. Advanced Structured Materials, 2020, , 199-216.	0.5	0
15	A New Pathology in the Simulation of Chaotic Dynamical Systems on Digital Computers. Advanced Theory and Simulations, 2019, 2, 1900125.	2.8	22
16	A Biophysical Model for Curvature-Guided Cell Migration. Biophysical Journal, 2019, 117, 1136-1144.	0.5	22
17	The Role of Graphene in Enhancing the Material Properties of Thermosetting Polymers. Advanced Theory and Simulations, 2019, 2, 1800168.	2.8	13
18	Multiscale modelling, simulation and computing: from the desktop to the exascale. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180355.	3.4	12

#	Article	IF	Citations
19	Multiscale computing for science and engineering in the era of exascale performance. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180144.	3.4	18
20	The heterogeneous multiscale method applied to inelastic polymer mechanics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180150.	3.4	12
21	Micromechanical exfoliation of graphene on the atomistic scale. Physical Chemistry Chemical Physics, 2019, 21, 5716-5722.	2.8	84
22	Grapheneâ€“Graphene Interactions: Friction, Superlubricity, and Exfoliation. Advanced Materials, 2018, 30, e1705791.	21.0	105
23	Curvotaxis directs cell migration through cell-scale curvature landscapes. Nature Communications, 2018, 9, 3995.	12.8	190
24	Chemically Specific Multiscale Modeling of the Shear-Induced Exfoliation of Clayâ€“Polymer Nanocomposites. ACS Omega, 2018, 3, 6439-6445.	3.5	8
25	Stem cell mechanical behaviour modelling: substrateâ€™s curvature influence during adhesion. Biomechanics and Modeling in Mechanobiology, 2017, 16, 1295-1308.	2.8	35
26	Multiscale computing in the exascale era. Journal of Computational Science, 2017, 22, 15-25.	2.9	54
27	Beam-particle approach to model cracking and energy dissipation in concrete: Identification strategy and validation. Cement and Concrete Composites, 2016, 70, 1-14.	10.7	20
28	On the calculation of equilibrium thermodynamic properties from molecular dynamics. Physical Chemistry Chemical Physics, 2016, 18, 30236-30240.	2.8	80
29	Lattice models applied to cyclic behavior description of quasiâ€brittle materials: advantages of implicit integration. International Journal for Numerical and Analytical Methods in Geomechanics, 2015, 39, 775-798.	3.3	11
30	Mechanism of Exfoliation and Prediction of Materials Properties of Clayâ€“Polymer Nanocomposites from Multiscale Modeling. Nano Letters, 2015, 15, 8108-8113.	9.1	45
31	Structure, Dynamics, and Function of the Hammerhead Ribozyme in Bulk Water and at a Clay Mineral Surface from Replica Exchange Molecular Dynamics. Langmuir, 2015, 31, 2493-2501.	3.5	16
32	Regularised crack behaviour effects on continuum modelling of quasi-brittle materials under cyclic loading. Engineering Fracture Mechanics, 2015, 149, 18-36.	4.3	17
33	Chemically Specific Multiscale Modeling of Clayâ€“Polymer Nanocomposites Reveals Intercalation Dynamics, Tactoid Selfâ€Assembly and Emergent Materials Properties. Advanced Materials, 2015, 27, 966-984.	21.0	98
34	Computing Clinically Relevant Binding Free Energies of HIV-1 Protease Inhibitors. Journal of Chemical Theory and Computation, 2014, 10, 1228-1241.	5.3	123
35	Clay Minerals Mediate Folding and Regioselective Interactions of RNA: A Large-Scale Atomistic Simulation Study. Journal of the American Chemical Society, 2010, 132, 13750-13764.	13.7	62
36	A critical appraisal of polymerâ€“clay nanocomposites. Chemical Society Reviews, 2008, 37, 568-594.	38.1	369

#	Article	IF	Citations
37	Identification of Constitutive Relationships for Concrete Using Discrete and Finite Element Framework. , 0, , .		0