Maxime Vassaux

List of Publications by Year
in descending order

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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	A critical appraisal of polymerâ€“clay nanocomposites. Chemical Society Reviews, 2008, 37, 568-594.	38.1	369
2	Curvotaxis directs cell migration through cell-scale curvature landscapes. Nature Communications, 2018, 9, 3995.	12.8	190
3	Computing Clinically Relevant Binding Free Energies of HIV-1 Protease Inhibitors. Journal of Chemical Theory and Computation, 2014, 10, 1228-1241.	5.3	123
4	Grapheneâ€“Graphene Interactions: Friction, Superlubricity, and Exfoliation. Advanced Materials, 2018, 30, e1705791.	21.0	105
5	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
6	Micromechanical exfoliation of graphene on the atomistic scale. Physical Chemistry Chemical Physics, 2019, 21, 5716-5722.	2.8	84
7	On the calculation of equilibrium thermodynamic properties from molecular dynamics. Physical Chemistry Chemical Physics, 2016, 18, 30236-30240.	2.8	80
8	Rapid, accurate, precise and reproducible ligandâ€“protein binding free energy prediction. Interface Focus, 2020, 10, 20200007.	3.0	77
9	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
10	Multiscale computing in the exascale era. Journal of Computational Science, 2017, 22, 15-25.	2.9	54
11	Mechanism of Exfoliation and Prediction of Materials Properties of Clayâ€“Polymer Nanocomposites from Multiscale Modeling. Nano Letters, 2015, 15, 8108-8113.	9.1	45
12	Uncertainty quantification in classical molecular dynamics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200082.	3.4	44
13	Stem cell mechanical behaviour modelling: substrateâ€™s curvature influence during adhesion. Biomechanics and Modeling in Mechanobiology, 2017, 16, 1295-1308.	2.8	35
14	EasyVVUQ: A Library for Verification, Validation and Uncertainty Quantification in High Performance Computing. Journal of Open Research Software, 2020, 8, 11.	5.9	34
15	Actomyosin, vimentin and LINC complex pull on osteosarcoma nuclei to deform on micropillar topography. Biomaterials, 2020, 234, 119746.	11.4	25
16	A New Pathology in the Simulation of Chaotic Dynamical Systems on Digital Computers. Advanced Theory and Simulations, 2019, 2, 1900125.	2.8	22
17	A Biophysical Model for Curvature-Guided Cell Migration. Biophysical Journal, 2019, 117, 1136-1144.	0.5	22
18	Building Confidence in Simulation: Applications of EasyVVUQ. Advanced Theory and Simulations, 2020, 3, 1900246.	2.8	21

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19	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
20	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
21	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
22	Regularised crack behaviour effects on continuum modelling of quasi-brittle materials under cyclic loading. Engineering Fracture Mechanics, 2015, 149, 18-36.	4.3	17
23	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
24	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
25	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
26	The Role of Graphene in Enhancing the Material Properties of Thermosetting Polymers. Advanced Theory and Simulations, 2019, 2, 1800168.	2.8	13
27	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
28	The heterogeneous multiscale method applied to inelastic polymer mechanics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180150.	3.4	12
29	Toward High Fidelity Materials Property Prediction from Multiscale Modeling and Simulation. Advanced Theory and Simulations, 2020, 3, 1900122.	2.8	12
30	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
31	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
32	Chemically Specific Multiscale Modeling of the Shear-Induced Exfoliation of Clayâ€“Polymer Nanocomposites. ACS Omega, 2018, 3, 6439-6445.	3.5	8
33	From digital hype to analogue reality: Universal simulation beyond the quantum and exascale eras. Journal of Computational Science, 2020, 46, 101093.	2.9	5
34	Hybrid parallelization of molecular dynamics simulations to reduce load imbalance. Journal of Supercomputing, 2022, 78, 9184-9215.	3.6	3
35	Accelerating Heterogeneous Multiscale Simulations of Advanced Materials Properties with Graphâ€Based Clustering. Advanced Theory and Simulations, 2021, 4, 2000234.	2.8	1
36	Identification of Constitutive Relationships for Concrete Using Discrete and Finite Element Framework. , 0, , .		0

#	Article	IF	Citations
37	Designing Optimal Scaffold Topographies to Promote Nucleus-Guided Mechanosensitive Cell Migration Using in Silico Models. Advanced Structured Materials, 2020, , 199-216.	0.5	0