James Kermode

List of Publications by Citations

34 papers	2,799 citations	17 h-index	37 g-index
37 ext. papers	3,457 ext. citations	6.3 avg, IF	5.22 L-index

#	Paper	IF	Citations
34	The atomic simulation environment-a Python library for working with atoms. *Journal of Physics Condensed Matter*, **2017**, 29, 273002	1.8	1097
33	Molecular dynamics with on-the-fly machine learning of quantum-mechanical forces. *Physical Review Letters*, **2015**, 114, 096405	7.4	362
32	Machine learning unifies the modeling of materials and molecules. *Science Advances*, **2017**, 3, e1701816	14.3	346
31	Low-speed fracture instabilities in a brittle crystal. *Nature*, **2008**, 455, 1224-1227	50.4	170
30	Understanding and mitigating hydrogen embrittlement of steels: a review of experimental, modelling and design progress from atomistic to continuum. *Journal of Materials Science*, **2018**, 53, 6251-6290	4.3	138
29	Hybrid atomistic simulation methods for materials systems. *Reports on Progress in Physics*, **2009**, 72, 026501	14.4	133
28	Machine Learning a General-Purpose Interatomic Potential for Silicon. *Physical Review X*, **2018**, 8,	9.1	122
27	Atomistic aspects of fracture. *International Journal of Fracture*, **2015**, 191, 13-30	2.3	98
26	In situ stable crack growth at the micron scale. *Nature Communications*, **2017**, 8, 108	17.4	33
25	Macroscopic scattering of cracks initiated at single impurity atoms. *Nature Communications*, **2013**, 4, 2441	17.4	33
24	Dissociative chemisorption of O2 inducing stress corrosion cracking in silicon crystals. *Physical Review Letters*, **2014**, 112, 115501	7.4	29
23	A framework for machine-learning-augmented multiscale atomistic simulations on parallel supercomputers. *International Journal of Quantum Chemistry*, **2015**, 115, 1129-1139	2.1	28
22	A universal preconditioner for simulating condensed phase materials. *Journal of Chemical Physics*, **2016**, 144, 164109	3.9	27
21	Development of an exchange□correlation functional with uncertainty quantification capabilities for density functional theory. *Journal of Computational Physics*, **2016**, 311, 173-195	4.1	26
20	A first principles based polarizable O(N) interatomic force field for bulk silica. *Journal of Chemical Physics*, **2010**, 133, 094102	3.9	22
19	Modelling defects in Ni□Al with EAM and DFT calculations. *Modelling and Simulation in Materials Science and Engineering*, **2016**, 24, 045012	2	18
18	Low Speed Crack Propagation via Kink Formation and Advance on the Silicon (110) Cleavage Plane. *Physical Review Letters*, **2015**, 115, 135501	7.4	17

17	Accuracy of buffered-force QM/MM simulations of silica. *Journal of Chemical Physics*, **2015**, 142, 064116	3.9	15
16	Sensitivity and dimensionality of atomic environment representations used for machine learning interatomic potentials. *Journal of Chemical Physics*, **2020**, 153, 144106	3.9	14
15	Validity of linear elasticity in the crack-tip region of ideal brittle solids. *International Journal of Fracture*, **2014**, 189, 103-110	2.3	13
14	Computing energy barriers for rare events from hybrid quantum/classical simulations through the virtual work principle. *Physical Review B*, **2017**, 96,	3.3	9
13	Imeall: A computational framework for the calculation of the atomistic properties of grain boundaries. *Computer Physics Communications*, **2018**, 232, 256-263	4.2	7
12	A preconditioning scheme for minimum energy path finding methods. *Journal of Chemical Physics*, **2019**, 150, 094109	3.9	5
11	Enabling QM-accurate simulation of dislocation motion in Ni and Fe using a hybrid multiscale approach. *Physical Review Materials*, **2019**, 3,	3.2	5
10	Efficient and transferable machine learning potentials for the simulation of crystal defects in bcc Fe and W. *Physical Review Materials*, **2021**, 5,	3.2	5
9	f90wrap: an automated tool for constructing deep Python interfaces to modern Fortran codes. *Journal of Physics Condensed Matter*, **2020**, 32, 305901	1.8	5
8	Hybrid quantum/classical study of hydrogen-decorated screw dislocations in tungsten: Ultrafast pipe diffusion, core reconstruction, and effects on glide mechanism. *Physical Review Materials*, **2020**, 4,	3.2	4
7	Multiscale Modeling of Defectsin Semiconductors:A Novel Molecular-Dynamics Scheme. *Topics in Applied Physics*, **2006**, 193-212	0.5	3
6	Atomistic QM/MM simulations of the strength of covalent interfaces in carbon nanotube-polymer composites. *Physical Chemistry Chemical Physics*, **2020**, 22, 12007-12014	3.6	2
5	Multiscale Modelling of Materials Chemomechanics: Brittle Fracture of Oxides and Semiconductors **2014**, 3, 1681-1686		2
4	Accelerating multiscale modelling of fluids with on-the-fly Gaussian process regression. *Microfluidics and Nanofluidics*, **2018**, 22, 139	2.8	2
3	Hybrid Quantum/Classical Modeling of Material Systems: The Learn on the Fly Molecular Dynamics Scheme. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 1-23	0.7	1
2	Numerical-continuation-enhanced flexible boundary condition scheme applied to mode-I and mode-III fracture. *Physical Review E*, **2021**, 103, 033002	2.4	1
1	Multiscale simulations of critical interfacial failure in carbon nanotube-polymer composites. *Journal of Chemical Physics*, **2018**, 149, 224102	3.9	1