John K Brennan

List of Publications by Year
in descending order

22 papers	595 citations	687363 13 h-index	713466 21 g-index
22 all docs	22 docs citations	22 times ranked	499 citing authors

#	Article	IF	Citations
1	An enhanced entangled polymer model for dissipative particle dynamics. Journal of Chemical Physics, 2012, 136, 134903.	3.0	114
2	A coarse-grain force field for RDX: Density dependent and energy conserving. Journal of Chemical Physics, 2016, 144, 104501.	3.0	61
3	Coarse-Grain Model Simulations of Nonequilibrium Dynamics in Heterogeneous Materials. Journal of Physical Chemistry Letters, 2014, 5, 2144-2149.	4.6	59
4	Dissipative particle dynamics at isothermal, isobaric, isoenergetic, and isoenthalpic conditions using Shardlow-like splitting algorithms. Journal of Chemical Physics, 2011, 135, 204105.	3.0	56
5	Mesoscale simulation of polymer reaction equilibrium: Combining dissipative particle dynamics with reaction ensemble Monte Carlo. I. Polydispersed polymer systems. Journal of Chemical Physics, 2006, 125, 164905.	3.0	55
6	Mesoscale simulation of polymer reaction equilibrium: Combining dissipative particle dynamics with reaction ensemble Monte Carlo. II. Supramolecular diblock copolymers. Journal of Chemical Physics, 2009, 130, 104902.	3.0	37
7	Parallel implementation of isothermal and isoenergetic Dissipative Particle Dynamics using Shardlow-like splitting algorithms. Computer Physics Communications, 2014, 185, 1987-1998.	7.5	30
8	Free-energy calculations using classical molecular simulation: application to the determination of the melting point and chemical potential of a flexible RDX model. Physical Chemistry Chemical Physics, 2016, 18, 7841-7850.	2.8	24
9	Generalised dissipative particle dynamics with energy conservation: density- and temperature-dependent potentials. Physical Chemistry Chemical Physics, 2019, 21, 24891-24911.	2.8	21
10	Dissipative particle dynamics with reactions: Application to RDX decomposition. Journal of Chemical Physics, 2019, 151, 114112.	3.0	20
11	Highly scalable discrete-particle simulations with novel coarse-graining: accessing the microscale. Molecular Physics, 2018, 116, 2061-2069.	1.7	16
12	Toward a Predictive Hierarchical Multiscale Modeling Approach for Energetic Materials. Challenges and Advances in Computational Chemistry and Physics, 2019, , 229-282.	0.6	16
13	LAMMPS integrated materials engine (LIME) for efficient automation of particle-based simulations: application to equation of state generation. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 055006.	2.0	14
14	CECAM Workshop: â€˜Dissipative particle dynamics: addressing deficiencies and establishing new frontiersâ€™ (16â€“18 July 2008, Lausanne, Switzerland). Molecular Simulation, 2009, 35, 766-769.	2.0	13
15	Forging of Hierarchical Multiscale Capabilities for Simulation of Energetic Materials. Propellants, Explosives, Pyrotechnics, 2020, 45, 177-195.	1.6	13
16	Coarse-grain modelling using an equation-of-state many-body potential: application to fluid mixtures at high temperature and high pressure. Molecular Physics, 2018, 116, 3271-3282.	1.7	12
17	Exponential-six potential scaling for the calculation of free energies in molecular simulations. Molecular Physics, 2015, 113, 45-54.	1.7	9
18	Generalized Energy-Conserving Dissipative Particle Dynamics with Reactions. Journal of Chemical Theory and Computation, 2022, 18, 2503-2512.	5.3	9

#	Article	IF	Citations
19	Generalized energy-conserving dissipative particle dynamics revisited: Insight from the thermodynamics of the mesoparticle leading to an alternative heat flow model. Physical Review E, 2021, 103, 062128.	2.1	8
20	Bottom-up coarse-grain modeling of nanoscale shear bands in shocked Î±-RDX. Journal of Materials Science, 2022, 57, 10627-10648.	3.7	5
21	Predicting Melt Curves of Energetic Materials Using Molecular Models. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.6	2
22	Toward Addressing the Challenge to Predict the Heat Capacities of RDX and HMX Energetic Materials. Propellants, Explosives, Pyrotechnics, 0, , .	1.6	1