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	Generalized Energy-Conserving Dissipative Particle Dynamics with Reactions. Journal of Chemical Theory and Computation, 2022, 18, 2503-2512.	5.3	9
2	Bottom-up coarse-grain modeling of nanoscale shear bands in shocked Î±-RDX. Journal of Materials Science, 2022, 57, 10627-10648.	3.7	5
3	Predicting Melt Curves of Energetic Materials Using Molecular Models. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.6	2
4	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
5	Forging of Hierarchical Multiscale Capabilities for Simulation of Energetic Materials. Propellants, Explosives, Pyrotechnics, 2020, 45, 177-195.	1.6	13
6	Dissipative particle dynamics with reactions: Application to RDX decomposition. Journal of Chemical Physics, 2019, 151, 114112.	3.0	20
7	Toward a Predictive Hierarchical Multiscale Modeling Approach for Energetic Materials. Challenges and Advances in Computational Chemistry and Physics, 2019, , 229-282.	0.6	16
8	Generalised dissipative particle dynamics with energy conservation: density- and temperature-dependent potentials. Physical Chemistry Chemical Physics, 2019, 21, 24891-24911.	2.8	21
9	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
10	Highly scalable discrete-particle simulations with novel coarse-graining: accessing the microscale. Molecular Physics, 2018, 116, 2061-2069.	1.7	16
11	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
12	A coarse-grain force field for RDX: Density dependent and energy conserving. Journal of Chemical Physics, 2016, 144, 104501.	3.0	61
13	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
14	Exponential-six potential scaling for the calculation of free energies in molecular simulations. Molecular Physics, 2015, 113, 45-54.	1.7	9
15	Parallel implementation of isothermal and isoenergetic Dissipative Particle Dynamics using Shardlow-like splitting algorithms. Computer Physics Communications, 2014, 185, 1987-1998.	7.5	30
16	Coarse-Grain Model Simulations of Nonequilibrium Dynamics in Heterogeneous Materials. Journal of Physical Chemistry Letters, 2014, 5, 2144-2149.	4.6	59
17	An enhanced entangled polymer model for dissipative particle dynamics. Journal of Chemical Physics, 2012, 136, 134903.	3.0	114
18	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

#	Article	IF	Citations
19	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
20	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
21	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
22	Toward Addressing the Challenge to Predict the Heat Capacities of RDX and HMX Energetic Materials. Propellants, Explosives, Pyrotechnics, 0, , .	1.6	1