

Jesse G Mcdaniel

List of Publications by Year in descending order

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42
papers

1,417
citations

304368

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329751

37
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docs citations

45
times ranked

1576
citing authors

#	ARTICLE	IF	CITATIONS
1	Physically-Motivated Force Fields from Symmetry-Adapted Perturbation Theory. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2053-2066.	1.1	120
2	Ab Initio, Physically Motivated Force Fields for CO ₂ Adsorption in Zeolitic Imidazolate Frameworks. <i>Journal of Physical Chemistry C</i> , 2012, 116, 1892-1903.	1.5	87
3	Evaluation of Force Field Performance for High-Throughput Screening of Gas Uptake in Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2015, 119, 3143-3152.	1.5	85
4	Ab Initio Force Fields for Imidazolium-Based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7024-7036.	1.2	76
5	Transferable Next-Generation Force Fields from Simple Liquids to Complex Materials. <i>Accounts of Chemical Research</i> , 2015, 48, 548-556.	7.6	71
6	First-Principles United Atom Force Field for the Ionic Liquid BMIM ⁺ BF ₄ ⁻ : An Alternative to Charge Scaling. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3560-3568.	1.2	68
7	Next-Generation Force Fields from Symmetry-Adapted Perturbation Theory. <i>Annual Review of Physical Chemistry</i> , 2016, 67, 467-488.	4.8	66
8	Ion Correlation and Collective Dynamics in BMIM/BF ₄ -Based Organic Electrolytes: From Dilute Solutions to the Ionic Liquid Limit. <i>Journal of Physical Chemistry B</i> , 2018, 122, 7154-7169.	1.2	60
9	First-Principles, Physically Motivated Force Field for the Ionic Liquid [BMIM][BF ₄]. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2670-2674.	2.1	57
10	Influence of Electronic Polarization on the Structure of Ionic Liquids. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4765-4770.	2.1	54
11	Robust, Transferable, and Physically Motivated Force Fields for Gas Adsorption in Functionalized Zeolitic Imidazolate Frameworks. <i>Journal of Physical Chemistry C</i> , 2012, 116, 14031-14039.	1.5	53
12	First-Principles Many-Body Force Fields from the Gas Phase to Liquid: A "Universal" Approach. <i>Journal of Physical Chemistry B</i> , 2014, 118, 8042-8053.	1.2	52
13	Physically Motivated, Robust, ab Initio Force Fields for CO ₂ and N ₂ . <i>Journal of Physical Chemistry B</i> , 2011, 115, 10054-10063.	1.2	51
14	Understanding the Properties of Ionic Liquids: Electrostatics, Structure Factors, and Their Sum Rules. <i>Journal of Physical Chemistry B</i> , 2019, 123, 3499-3512.	1.2	48
15	Ab Initio Force Fields for Organic Anions: Properties of [BMIM][TFSI], [BMIM][FSI], and [BMIM][OTf] Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4101-4114.	1.2	45
16	Polarization Effects in Binary [BMIM ⁺][BF ₄ ⁻]/1,2-Dichloroethane, Acetone, Acetonitrile, and Water Electrolytes. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4345-4355.	1.2	33
17	On the Miscibility and Immiscibility of Ionic Liquids and Water. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5343-5356.	1.2	29
18	Proper Thermal Equilibration of Simulations with Drude Polarizable Models: Temperature-Grouped Dual-Nosé-Hoover Thermostat. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7523-7530.	2.1	29

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19	Interference of electrical double layers: Confinement effects on structure, dynamics, and screening of ionic liquids. <i>Journal of Chemical Physics</i> , 2020, 152, 074709.	1.2	29
20	A nanoconfined iron(III) fluoride cathode in a NaDFOB electrolyte: towards high-performance sodium-ion batteries. <i>Journal of Materials Chemistry A</i> , 2020, 8, 4091-4098.	5.2	28
21	Inner Layer Capacitance of Organic Electrolytes from Constant Voltage Molecular Dynamics. <i>Journal of Physical Chemistry C</i> , 2020, 124, 2907-2922.	1.5	25
22	Tuning Water Networks via Ionic Liquid/Water Mixtures. <i>International Journal of Molecular Sciences</i> , 2020, 21, 403.	1.8	23
23	Conformational and Dynamic Properties of Poly(ethylene oxide) in an Ionic Liquid: Development and Implementation of a First-Principles Force Field. <i>Journal of Physical Chemistry B</i> , 2016, 120, 231-243.	1.2	21
24	Microscopic Origins of Enhanced Gas Adsorption and Selectivity in Mixed-Linker Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17131-17142.	1.5	20
25	Grotthuss Transport of Iodide in EMIM/1,3 Ionic Crystal. <i>Journal of Physical Chemistry B</i> , 2018, 122, 250-257.	1.2	17
26	Electrostatic Interactions Govern Odd/Even-Effects in Water-Induced Gemini Surfactant Self-Assembly. <i>Journal of Physical Chemistry B</i> , 2017, 121, 565-576.	1.2	16
27	Conformational and Dynamic Properties of Poly(ethylene oxide) in BMIM ⁺ BF ₄ ⁻ : A Microsecond Computer Simulation Study Using ab Initio Force Fields. <i>Macromolecules</i> , 2018, 51, 5336-5345.	2.2	16
28	Structure-Capacitance Relationships of Graphene/Ionic Liquid Electrolyte Double Layers. <i>Journal of Physical Chemistry C</i> , 2021, 125, 20204-20218.	1.5	16
29	Comment on "Isolating the non-polar contributions to the intermolecular potential for water-alkane interactions". <i>J. Chem. Phys.</i> 141, 064905 (2014)]. <i>Journal of Chemical Physics</i> , 2016, 144, 137101.	1.2	14
30	Deep Eutectic Solvents: Molecular Simulations with a First-Principles Polarizable Force Field. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7177-7186.	1.2	13
31	Dynamics of Water in Gemini Surfactant-Based Lyotropic Liquid Crystals. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10860-10868.	1.2	12
32	A Transferable Polarizable Force Field for Urea Crystals and Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7475-7483.	1.2	12
33	An efficient multi-scale lattice model approach to screening nano-porous adsorbents. <i>Journal of Chemical Physics</i> , 2012, 137, 244102.	1.2	11
34	Free energy barriers for TMEA ⁺ , TMA ⁺ , and BF ₄ ⁻ ion diffusion through nanoporous carbon electrodes. <i>Carbon</i> , 2020, 161, 550-561.	5.4	11
35	Capacitance of Carbon Nanotube/Graphene Composite Electrodes with [BMIM ⁺][BF ₄ ⁻]/Acetonitrile: Fixed Voltage Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5822-5837.	1.5	10
36	Importance of hydrophobic traps for proton diffusion in lyotropic liquid crystals. <i>Journal of Chemical Physics</i> , 2016, 144, 094705.	1.2	6

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37	Proton Transport in [BMIM ⁺][BF ₄ ⁻]/Water Mixtures Near the Percolation Threshold. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5957-5970.	1.2	6
38	Physics-based, neural network force fields for reactive molecular dynamics: Investigation of carbene formation from [EMIM ⁺][OAc ⁻]. <i>Journal of Chemical Physics</i> , 2021, 155, 104112.	1.2	6
39	DFT-based QM/MM with particle-mesh Ewald for direct, long-range electrostatic embedding. <i>Journal of Chemical Physics</i> , 2022, 156, 174105.	1.2	6
40	Quantized Electrodes: Atomic Palladium and Gold in Polyaniline. <i>ChemElectroChem</i> , 2021, 8, 1766-1774.	1.7	4
41	Coupling between the Dynamics of Water and Surfactants in Lyotropic Liquid Crystals. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5048-5057.	1.2	3
42	Proton Diffusion through Bilayer Pores. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9247-9259.	1.2	2