Luke Wylie

List of Publications by Year
in descending order

69 papers	3,221 citations	159358 30 h-index	149479 56 g-index
73 all docs	73 docs citations	73 times ranked	3103 citing authors

#	Article	IF	Citations
1	A <scp>DLPNOâ€CCSD</scp>(T) benchmarking study of intermolecular interactions of ionic liquids. Journal of Computational Chemistry, 2022, 43, 106-120.	1.5	6
2	Behavior of counterpoise correction in manyâ€body molecular clusters of organic compounds: <scp>Hartreeâ€“Fock</scp> interaction energy perspective. Journal of Computational Chemistry, 2022, 43, 568-576.	1.5	5
3	Inclusion of More Physics Leads to Less Data: Learning the Interaction Energy as a Function of Electron Deformation Density with Limited Training Data. Journal of Chemical Theory and Computation, 2022, 18, 1607-1618.	2.3	5
4	Prediction of lattice energy of benzene crystals: A robust theoretical approach. Journal of Computational Chemistry, 2021, 42, 248-260.	1.5	12
5	Electrochemical characterization and thermodynamic analysis of TEMPO derivatives in ionic liquids. Physical Chemistry Chemical Physics, 2021, 23, 10205-10217.	1.3	13
6	Experimental Evidence of Long-Lived Electric Fields of Ionic Liquid Bilayers. Journal of the American Chemical Society, 2021, 143, 17431-17440.	6.6	31
7	Establishing the accuracy of density functional approaches for the description of noncovalent interactions in ionic liquids. Physical Chemistry Chemical Physics, 2021, 23, 25558-25564.	1.3	5
8	A new twist on an old molecule: a rotameric isomer of bis(pentafluorophenyl)mercury. Journal of Coordination Chemistry, 2021, 74, 2947-2958.	0.8	1
9	Predicting Entropic Effects of Water Mixing with Ionic Liquids Containing Anions of Strong Hydrogen Bonding Ability: Role of the Cation. Journal of Physical Chemistry B, 2020, 124, 9182-9194.	1.2	4
10	Reversible Reduction of the TEMPO Radical: One Step Closer to an All-Organic Redox Flow Battery. ACS Sustainable Chemistry and Engineering, 2020, 8, 17988-17996.	3.2	37
11	A Systematic Study of DFT Performance for Geometry Optimizations of Ionic Liquid Clusters. Journal of Chemical Theory and Computation, 2020, 16, 6735-6753.	2.3	32
12	The effect of descriptor choice in machine learning models for ionic liquid melting point prediction. Journal of Chemical Physics, 2020, 153, 104101.	1.2	29
13	Isomers of Alkali Metal (Methylbenzyl)allylamides: A Theoretical Perspective. ACS Omega, 2020, 5, 9448-9457.	1.6	3
14	Ordered Solvents and Ionic Liquids Can Be Harnessed for Electrostatic Catalysis. Journal of the American Chemical Society, 2020, 142, 12826-12833.	6.6	37
15	Toward Improved Performance of All-Organic Nitroxide Radical Batteries with Ionic Liquids: A Theoretical Perspective. ACS Sustainable Chemistry and Engineering, 2019, 7, 5367-5375.	3.2	27
16	Increased stability of nitroxide radicals in ionic liquids: more than a viscosity effect. Physical Chemistry Chemical Physics, 2019, 21, 2882-2888.	1.3	18
17	Influence of DFT Functionals and Solvation Models on the Prediction of Far-Infrared Spectra of Pt-Based Anticancer Drugs: Why Do Different Complexes Require Different Levels of Theory?. ACS Omega, 2019, 4, 5254-5269.	1.6	5
18	An ab initio Study of the Structure and Energetics of Hydrogen Bonding in Ionic Liquids. Frontiers in Chemistry, 2019, 7, 208.	1.8	48

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19	Cluster approach to the prediction of thermodynamic and transport properties of ionic liquids. Journal of Chemical Physics, 2018, 148, 193832.	1.2	11
20	Anisotropic Thermal and Guestâ€Induced Responses of an Ultramicroporous Framework with Rigid Linkers. Chemistry - A European Journal, 2018, 24, 4774-4779.	1.7	3
21	Cellulose-dissolving protic ionic liquids as low cost catalysts for direct transesterification reactions of cellulose. Green Chemistry, 2018, 20, 1412-1422.	4.6	52
22	Spectroscopic Studies on Photoinduced Reactions of the Anticancer Prodrug, trans,trans,transâ€[Pt(N₃)₂(OH)₂(py)₂]. Chemistry - A European Journal, 2018, 24, 5790-5803.	1.7	31
23	Frontispiece: Anisotropic Thermal and Guest-Induced Responses of an Ultramicroporous Framework with Rigid Linkers. Chemistry - A European Journal, 2018, 24, .	1.7	0
24	Spectroscopic Studies on Photoinduced Reactions of the Anticancer Prodrug, trans,trans,trans -[Pt(N3)2 (OH)2 (py)2]. Chemistry - A European Journal, 2018, 24, 5679-5679.	1.7	0
25	Contrasting Synergistic Heterobimetallic (Naâ€“Mg) and Homometallic (Na or Mg) Bases in Metallation Reactions of Dialkylphenylphosphines and Dialkylanilines: Lateral versus Ring Selectivities. Chemistry - A European Journal, 2018, 24, 15669-15677.	1.7	8
26	Is it possible to control kinetic rates of radical polymerisation in ionic liquids?. Chemical Communications, 2018, 54, 11226-11243.	2.2	14
27	Structural changes in coordination polymers in response to small changes in steric bulk (H vs.) Tj ETQq1 1 0.784314 rgBT /Ove	1.3	31
28	Quantum Chemical Methods for the Prediction of Energetic, Physical, and Spectroscopic Properties of Ionic Liquids. Chemical Reviews, 2017, 117, 6696-6754.	23.0	181
29	Generalized spin-ratio scaled MP2 method for accurate prediction of intermolecular interactions for neutral and ionic species. Journal of Chemical Physics, 2017, 146, 064108.	1.2	34
30	Difference in chemical bonding between lithium and sodium salts: influence of covalency on their solubility. Physical Chemistry Chemical Physics, 2017, 19, 17366-17372.	1.3	22
31	Trends in Two- and Three-Body Effects in Multiscale Clusters of Ionic Liquids. Journal of Physical Chemistry B, 2017, 121, 577-588.	1.2	19
32	Application of spin-ratio scaled MP2 for the prediction of intermolecular interactions in chemical systems. Physical Chemistry Chemical Physics, 2017, 19, 28936-28942.	1.3	21
33	An improved model for malaria pigment and Î² â€hematin: Fe(OEP)picrate. Journal of Raman Spectroscopy, 2017, 48, 1148-1157.	1.2	1
34	Prediction of ¹H NMR chemical shifts for clusters of imidazolium-based ionic liquids. Physical Chemistry Chemical Physics, 2017, 19, 17411-17425.	1.3	33
35	Unusual Products from Oxidation of Naphthalene Diimides. Asian Journal of Organic Chemistry, 2016, 5, 490-493.	1.3	10
36	Comparison of the Effective Fragment Potential Method with Symmetry-Adapted Perturbation Theory in the Calculation of Intermolecular Energies for Ionic Liquids. Journal of Chemical Theory and Computation, 2016, 12, 2553-2568.	2.3	19

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37	Mechanisms of low temperature capture and regeneration of CO₂ using diamino protic ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 1140-1149.	1.3	42
38	Active space and basis set effects in <scp>CASPT</scp>2 models of the 1,3â€butadieneâ€ethene cycloaddition and the 1,3â€butadiene dimerization. International Journal of Quantum Chemistry, 2015, 115, 989-1001.	1.0	4
39	Novel SCS-IL-MP2 and SOS-IL-MP2 Methods for Accurate Energetics of Large-Scale Ionic Liquid Clusters. Journal of Chemical Theory and Computation, 2015, 11, 3610-3616.	2.3	15
40	Physical Absorption Of CO₂ in Protic and Aprotic Ionic Liquids: An Interaction Perspective. Journal of Physical Chemistry B, 2015, 119, 11748-11759.	1.2	50
41	Importance of dispersion forces for prediction of thermodynamic and transport properties of some common ionic liquids. Physical Chemistry Chemical Physics, 2014, 16, 7209-7221.	1.3	102
42	New SCS- and SOS-MP2 Coefficients Fitted to Semi-Coulombic Systems. Journal of Chemical Theory and Computation, 2014, 10, 3111-3122.	2.3	29
43	Anionâ€“Anion Interactions in the Crystal Packing of Functionalized Methanide Anions: An Experimental and Computational Study. Crystal Growth and Design, 2014, 14, 1922-1932.	1.4	25
44	A Redox Switchable Dihydrobenzo[b]pyrazine Pushâ€Pull System. Asian Journal of Organic Chemistry, 2014, 3, 619-623.	1.3	11
45	Experimental and theoretical studies of tetramethoxy-p-benzoquinone: infrared spectra, structural and lithium insertion properties. RSC Advances, 2013, 3, 19081.	1.7	21
46	Assessment of Kohnâ€“Sham density functional theory and MÃ¸llerâ€“Plesset perturbation theory for ionic liquids. Physical Chemistry Chemical Physics, 2013, 15, 13664.	1.3	98
47	Assessment of atomic partial charge schemes for polarisation and charge transfer effects in ionic liquids. Physical Chemistry Chemical Physics, 2013, 15, 1632-1646.	1.3	89
48	Large-scale ab initio calculations of archetypical ionic liquids. Chemical Communications, 2012, 48, 1493-1495.	2.2	43
49	A supramolecular twist to the structures of bis(polyfluorophenyl)mercurials. CrystEngComm, 2011, 13, 88-92.	1.3	5
50	Understanding the Effect of the C2 Proton in Promoting Low Viscosities and High Conductivities in Imidazolium-Based Ionic Liquids: Part I. Weakly Coordinating Anions. Journal of Physical Chemistry B, 2011, 115, 14688-14697.	1.2	101
51	Nature of Hydrogen Bonding in Charged Hydrogen-Bonded Complexes and Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2011, 115, 14659-14667.	1.2	132
52	Towards large-scale, fully ab initio calculations of ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 4189.	1.3	121
53	First Principles Prediction of The Propagation Rate Coefficients of Acrylic and Vinyl Esters: Are We There Yet?. Macromolecules, 2010, 43, 553-560.	2.2	66
54	New Insights into the Relationship between Ion-Pair Binding Energy and Thermodynamic and Transport Properties of Ionic Liquids. Journal of Physical Chemistry C, 2010, 114, 20472-20478.	1.5	81

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55	Theoretical and Experimental Insights into the Mechanism of the Nucleophilic Addition of Water and Methanol to Dicyanonitrosomethanide. Journal of Physical Chemistry B, 2010, 114, 16517-16527.	1.2	22
56	Ion-Pair Binding Energies of Ionic Liquids: Can DFT Compete with Ab Initio-Based Methods?. Journal of Physical Chemistry A, 2009, 113, 7064-7072.	1.1	163
57	The Madelung Constant of Organic Salts. Crystal Growth and Design, 2009, 9, 4834-4839.	1.4	64
58	On the components of the dielectric constants of ionic liquids: ionic polarization?. Physical Chemistry Chemical Physics, 2009, 11, 2452.	1.3	171
59	Energy-directed tree search: an efficient systematic algorithm for finding the lowest energy conformation of molecules. Physical Chemistry Chemical Physics, 2007, 9, 2507.	1.3	49
60	Should Contemporary Density Functional Theory Methods Be Used to Study the Thermodynamics of Radical Reactions?. Journal of Physical Chemistry A, 2007, 111, 10754-10768.	1.1	140
61	An Ab Initio Guide to Structureâ€”Reactivity Trends in Reversible Addition Fragmentation Chain Transfer Polymerization. ACS Symposium Series, 2006, , 406-420.	0.5	25
62	Radical Addition to Thioketones:â€‰ Computer-Aided Design of Spin Traps for Controlling Free-Radical Polymerization. Journal of Chemical Theory and Computation, 2006, 2, 1632-1645.	2.3	27
63	Addition-Fragmentation Kinetics of Fluorodithioformates (F-RAFT) in Styrene, Vinyl Acetate, and Ethylene Polymerization:Â An Ab Initio Investigation. Macromolecules, 2006, 39, 4585-4591.	2.2	55
64	Reliable Low-Cost Theoretical Procedures for Studying Additionâ€“Fragmentation in RAFT Polymerization. Journal of Physical Chemistry A, 2006, 110, 2486-2492.	1.1	85
65	Accurate ab initio prediction of propagation rate coefficients in free-radical polymerization: Acrylonitrile and vinyl chloride. Chemical Physics, 2006, 324, 96-110.	0.9	136
66	Computational Studies of RAFT Polymerizationâ€“Mechanistic Insights and Practical Applications. Macromolecular Rapid Communications, 2006, 27, 473-497.	2.0	122
67	Quantum Chemical Mapping of Initialization Processes in RAFT Polymerization. Macromolecular Rapid Communications, 2006, 27, 1015-1022.	2.0	67
68	Is the Addition-Fragmentation Step of the RAFT Polymerisation Process Chain Length Dependent?. Macromolecular Theory and Simulations, 2006, 15, 394-403.	0.6	44
69	Trends in Râ€“X Bond Dissociation Energies (R = Me, Et,i-Pr,t-Bu; X = H, CH3, OCH3, OH, F):Â A Surprising Shortcoming of Density Functional Theory. Journal of Physical Chemistry A, 2005, 109, 7558-7566.	1.1	210