Christoffer Heath Turner

List of Publications by Year
in descending order

98	2,599	186265	223800
papers	citations	28 h-index	46 g-index

101	101	101	3414
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Effect of confinement on chemical reaction equilibria: The reactions 2NOâ‡”(NO)2 and N2+3H2â‡”2NH3 in carbon micropores. Journal of Chemical Physics, 2001, 114, 1851-1859.	3.0	106
2	Simulation of chemical reaction equilibria by the reaction ensemble Monte Carlo method: a reviewâ€. Molecular Simulation, 2008, 34, 119-146.	2.0	102
3	The Critical Role of Surfactants in the Growth of Cobalt Nanoparticles. Langmuir, 2010, 26, 478-483.	3.5	95
4	Hydrodeoxygenation of m-cresol over bimetallic NiFe alloys: Kinetics and thermodynamics insight into reaction mechanism. Journal of Catalysis, 2018, 359, 272-286.	6.2	95
5	First-principles study of methane dehydrogenation on a bimetallic Cu/Ni(111) surface. Journal of Chemical Physics, 2009, 131, 174702.	3.0	94
6	Synthesis and Growth Mechanism of Iron Oxide Nanowhiskers. Nano Letters, 2011, 11, 1141-1146.	9.1	92
7	Adsorption and catalysis: The effect of confinement on chemical reactions. Applied Surface Science, 2005, 252, 766-777.	6.1	85
8	Catalytic activity of bimetallic nickel alloys for solid-oxide fuel cell anode reactions from density-functional theory. Journal of Power Sources, 2011, 196, 4724-4728.	7.8	84
9	Chemisorption of Transition-Metal Atoms on Boron- and Nitrogen-Doped Carbon Nanotubes: Energetics and Geometric and Electronic Structures. Journal of Physical Chemistry C, 2009, 113, 7069-7078.	3.1	71
10	Effect of confinement by porous materials on chemical reaction kinetics. Journal of Chemical Physics, 2002, 116, 2138-2148.	3.0	67
11	Linking Carbon and Boron-Nitride Nanotubes: Heterojunction Energetics and Band Gap Tuning. Journal of Physical Chemistry Letters, 2010, 1, 2269-2273.	4.6	67
12	Characterizing the Interaction of Pt and PtRu Clusters with Boron-Doped, Nitrogen-Doped, and Activated Carbon: Density Functional Theory Calculations and Parameterization. Journal of Physical Chemistry C, 2008, 112, 13607-13622.	3.1	60
13	Chemical and Physical Absorption of SO₂ by N-Functionalized Imidazoles: Experimental Results and Molecular-level Insight. Industrial & Engineering Chemistry Research, 2015, 54, 462-471.	3.7	60
14	Boron-doped carbon powders formed at 1000Â°C and one atmosphere. Carbon, 2008, 46, 1711-1717.	10.3	59
15	Hydrodeoxygenation of guaiacol over bimetallic Fe-alloyed (Ni, Pt) surfaces: reaction mechanism, transition-state scaling relations and descriptor for predicting Câ€“O bond scission reactivity. Catalysis Science and Technology, 2018, 8, 2146-2158.	4.1	56
16	Effect of boron doping in the carbon support on platinum nanoparticles and carbon corrosion. Journal of Power Sources, 2009, 192, 324-329.	7.8	51
17	Influence of chemical and physical surface heterogeneity on chemical reaction equilibria in carbon micropores. Molecular Physics, 2001, 99, 1991-2001.	1.7	50
18	Stabilization of Platinum Clusters by Substitutional Boron Dopants in Carbon Supports. Journal of Physical Chemistry B, 2006, 110, 17706-17710.	2.6	50

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19	Mechanism of Bismuth Telluride Exfoliation in an Ionic Liquid Solvent. Langmuir, 2015, 31, 3644-3652.	3.5	45
20	Initial Surface Reactions of TiO2Atomic Layer Deposition onto SiO2Surfaces:Â Density Functional Theory Calculations. Journal of Physical Chemistry B, 2006, 110, 8337-8347.	2.6	40
21	Effects of supercritical clustering and selective confinement on reaction equilibrium: A molecular simulation study of the esterification reaction. Journal of Chemical Physics, 2003, 119, 6057-6067.	3.0	38
22	Atomic Layer Deposition of TiO2from TiI4and H2O onto SiO2Surfaces:Â Ab Initio Calculations of the Initial Reaction Mechanisms. Journal of the American Chemical Society, 2007, 129, 3863-3878.	13.7	38
23	Structure and reactivity of single site Ti catalysts for propylene epoxidation. Journal of Catalysis, 2019, 377, 419-428.	6.2	38
24	Electronic structure calculations of gas adsorption on boron-doped carbon nanotubes sensitized with tungsten. Chemical Physics Letters, 2009, 482, 274-280.	2.6	37
25	Effects of TiO₂ in Low Temperature Propylene Epoxidation Using Gold Catalysts. Journal of Physical Chemistry C, 2018, 122, 1688-1698.	3.1	37
26	Molecular Simulation of Ionic Polyimides and Composites with Ionic Liquids as Gas-Separation Membranes. Langmuir, 2017, 33, 11377-11389.	3.5	36
27	Adsorption properties of nitrogen dioxide on hybrid carbon and boron-nitride nanotubes. Physical Chemistry Chemical Physics, 2014, 16, 22853-22860.	2.8	31
28	Confinement Effects on Carbon Dioxide Methanation: A Novel Mechanism for Abiotic Methane Formation. Scientific Reports, 2017, 7, 9021.	3.3	31
29	Molecular dynamics simulation of the Al₂O₃film structure during atomic layer deposition. Molecular Simulation, 2009, 35, 270-279.	2.0	28
30	3D Printed Block Copolymer Nanostructures. Journal of Chemical Education, 2015, 92, 1866-1870.	2.3	28
31	1,2,3-Trimethoxypropane: A Glycerol-Derived Physical Solvent for CO₂ Absorption. ACS Sustainable Chemistry and Engineering, 2017, 5, 911-921.	6.7	28
32	Molecular insight into the anion effect and free volume effect of CO₂solubility in multivalent ionic liquids. Physical Chemistry Chemical Physics, 2020, 22, 20618-20633.	2.8	27
33	Molecular Simulation of the Thermophysical Properties of N-Functionalized Alkylimidazoles. Journal of Physical Chemistry B, 2012, 116, 6529-6535.	2.6	26
34	Electrostatic Potential within the Free Volume Space of Imidazole-Based Solvents: Insights into Gas Absorption Selectivity. Journal of Physical Chemistry B, 2014, 118, 255-264.	2.6	26
35	Mechanistic insights into the direct propylene epoxidation using Au nanoparticles dispersed on TiO2/SiO2. Chemical Engineering Science, 2018, 191, 169-182.	3.8	26
36	Formation mechanism and composition distribution of FePt nanoparticles. Journal of Applied Physics, 2007, 102, 104310.	2.5	25

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37	Molecular analysis of selective gas adsorption within composites of ionic polyimides and ionic liquids as gas separation membranes. Chemical Physics, 2019, 516, 71-83.	1.9	25
38	Platinum attachments on iron oxide nanoparticle surfaces. Journal of Applied Physics, 2010, 107, 09B311.	2.5	24
39	Relationship between pore size and reversible and irreversible immobilization of ionic liquid electrolytes in porous carbon under applied electric potential. Applied Physics Letters, 2016, 109, .	3.3	23
40	Theoretical Studies on the Direct Propylene Epoxidation Using Gold-Based Catalysts: A Mini-Review. Catalysts, 2018, 8, 421.	3.5	21
41	Structural and Electronic Properties of Carbon Nanotubes and Graphenes Functionalized with Cyclopentadienylâ€“Transition Metal Complexes: A DFT Study. Journal of Physical Chemistry C, 2013, 117, 8758-8766.	3.1	20
42	Modeling the atomistic growth behavior of gold nanoparticles in solution. Nanoscale, 2016, 8, 9354-9365.	5.6	20
43	Analysis of the propylene epoxidation mechanism on supported gold nanoparticles. Chemical Engineering Science, 2017, 174, 229-237.	3.8	20
44	Screening Ionic Liquids Based on Ionic Volume and Electrostatic Potential Analyses. Journal of Physical Chemistry B, 2021, 125, 3653-3664.	2.6	20
45	Synthesis of 1,2-Dialkyl-, 1,4(5)-Dialkyl-, and 1,2,4(5)-Trialkylimidazoles via a One-Pot Method. Industrial & Engineering Chemistry Research, 2013, 52, 11880-11887.	3.7	19
46	Kinetic Monte Carlo simulation of the elementary electrochemistry in a hydrogen-powered solid oxide fuel cell. Journal of Power Sources, 2010, 195, 4177-4184.	7.8	18
47	Molecular Transport Behavior of CO₂ in Ionic Polyimides and Ionic Liquid Composite Membrane Materials. Journal of Physical Chemistry B, 2019, 123, 7455-7463.	2.6	18
48	The Nitric Oxide Dimer Reaction in Carbon Nanopores. Journal of Physical Chemistry B, 2018, 122, 3604-3614.	2.6	17
49	Solubility Behavior of CO₂ in Ionic Liquids Based on Ionic Polarity Index Analyses. Journal of Physical Chemistry B, 2021, 125, 3665-3676.	2.6	17
50	Oxygen reduction reaction on Pt(1â€¯1â€¯1), Pt(2â€¯2â€¯1), and Ni/Au1Pt3(2â€¯2â€¯1) surfaces: Probing scaling relationships of reaction energetics and interfacial composition. Chemical Engineering Science, 2018, 184, 239-250.	3.8	16
51	Solubility and diffusivity of CO2 in ionic polyimides with [C(CN)3]x[oAc]1â”x anion composition. Computational Materials Science, 2020, 174, 109468.	3.0	16
52	Molecular-level behavior of imidazolium-based ionic liquid mixtures. Chemical Engineering Science, 2021, 229, 116073.	3.8	16
53	Synthesis and Properties of 1,2,3-Triethoxypropane: A Glycerol-Derived Green Solvent Candidate. Industrial & Engineering Chemistry Research, 2020, 59, 20190-20200.	3.7	15
54	Tuning the Adsorption Interactions of Imidazole Derivatives with Specific Metal Cations. Journal of Physical Chemistry A, 2014, 118, 3944-3951.	2.5	14

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55	High-salinity brine desalination with amine-based temperature swing solvent extraction: A molecular dynamics study. Journal of Molecular Liquids, 2021, 341, 117359.	4.9	14
56	Replica Exchange for Reactive Monte Carlo Simulations. Journal of Physical Chemistry C, 2007, 111, 15706-15715.	3.1	13
57	Oxygen adsorption characteristics on hybrid carbon and boronâ€nitride nanotubes. Journal of Computational Chemistry, 2014, 35, 1058-1063.	3.3	13
58	Molecular Dynamics Simulation of Bismuth Telluride Exfoliation Mechanisms in Different Ionic Liquid Solvents. Langmuir, 2016, 32, 9982-9992.	3.5	13
59	An Atomistic Carbide-Derived Carbon Model Generated Using ReaxFF-Based Quenched Molecular Dynamics. Journal of Carbon Research, 2017, 3, 32.	2.7	13
60	Transition-Metal Strings Templated on Boron-Doped Carbon Nanotubes: A DFT Investigation. Journal of Physical Chemistry C, 2009, 113, 15346-15354.	3.1	12
61	DFT study on the effect of exocyclic substituents on the proton affinity of 1-methylimidazole. Chemical Physics, 2013, 416, 21-25.	1.9	12
62	Molecular aspects of temperature swing solvent extraction for brine desalination using imidazole-based solvents. Chemical Engineering Science, 2022, 247, 116866.	3.8	12
63	Computational and experimental study of different brines in temperature swing solvent extraction desalination with amine solvents. Desalination, 2022, 537, 115863.	8.2	12
64	Does solvent density play a role in the ketoâ€“enol tautomerism of acetylacetone?. Journal of Supercritical Fluids, 2006, 37, 201-208.	3.2	11
65	Kinetic Monte Carlo simulation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si72.gif" display="inline" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mtext>O</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msup></mml:mrow></mml:math> incorporation in the yttria stabilized zirconia (YSZ) fuel cell. Chemical Physics Letters, 2009, 471, 326-330.	2.6	11
66	Properties of symmetric 1,3-diethers based on glycerol skeletons for CO2 absorption. Fluid Phase Equilibria, 2020, 521, 112718.	2.5	11
67	Oxygen Incorporation Mechanism during Atomic Layer Deposition of Al2O3onto H-Passivated Si(100)-2Ã—1. Journal of Physical Chemistry C, 2007, 111, 5756-5759.	3.1	10
68	Molecular Simulation of High-Salinity Brines in Contact with Diisopropylamine and Tripropylamine Solvents. Industrial & Engineering Chemistry Research, 2021, 60, 7917-7925.	3.7	10
69	Monte Carlo Simulation of Formic Acid Dimerization in a Carbon Dioxide Solvent. Journal of Physical Chemistry B, 2004, 108, 11716-11721.	2.6	9
70	Molecular-level analysis of the wetting behavior of imidazolium-based ionic liquids on bismuth telluride surfaces. Chemical Engineering Science, 2020, 211, 115270.	3.8	9
71	Understanding Gas Solubility of Pure Component and Binary Mixtures within Multivalent Ionic Liquids from Molecular Simulations. Journal of Physical Chemistry B, 2021, 125, 8165-8174.	2.6	9
72	Synthesis and Properties of Symmetric Glycerol-Derived 1,2,3-Triethers and 1,3-Diether-2-Ketones for CO2 Absorption. Chemical Engineering Science, 2021, 248, 117150.	3.8	9

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73	Computational study of the electrostatic potential and charges of multivalent ionic liquid molecules. Journal of Molecular Liquids, 2021, 340, 117190.	4.9	9
74	Monte Carlo Simulation of Equilibrium Reactions at Vaporâ"Liquid Interfaces. Journal of Physical Chemistry B, 2005, 109, 23588-23595.	2.6	8
75	One-Dimensional Ni-Based Nanostructures and Their Application as Solid Oxide Fuel Cell Anodes: A DFT Investigation. Journal of Physical Chemistry C, 2013, 117, 1315-1322.	3.1	8
76	Redox Properties of Graphenes Functionalized with Cyclopentadieneâ€"Transition Metal Complexes: A Potential Redox-Active Material. Journal of Physical Chemistry C, 2014, 118, 24633-24640.	3.1	8
77	Molecular simulation of the separation of toluene and p-xylene with the thermally-robust ionic liquid triphenyl-p-phenyl sulfonyl phenyl phosphonium. Chemical Engineering Science, 2020, 224, 115790.	3.8	8
78	Glycerolâ€derived Solvents Containing Two or Three Distinct Functional Groups Enabled by Trifluoroethyl Glycidyl Ether. AICHE Journal, 0, , e17533.	3.6	8
79	Charge scaling parameter evaluation for multivalent ionic liquids with fixed point charge force fields. Journal of Ionic Liquids, 2022, 2, 100020.	2.7	8
80	Monte Carlo Simulation of Equilibrium Reactions at Modified Vaporâ"Liquid Interfaces. Langmuir, 2007, 23, 2525-2530.	3.5	7
81	Understanding gas absorption in multivalent ionic liquids via solute-solvent interaction analyses. Chemical Physics Letters, 2022, 786, 139204.	2.6	7
82	Enhancing the pre-polymerization coordination of 1-vinylimidazole. Chemical Engineering Science, 2015, 138, 646-654.	3.8	6
83	Photopolymerization Behavior of Coordinated Ionic Liquids Formed from Organic Monomers with Alkali and Alkaline Earth Metal Bistriflimide Salts. Macromolecular Chemistry and Physics, 2017, 218, 1600358.	2.2	6
84	Structural, electronic, and magnetic features of platinum alloy strings templated on a boron-doped carbon nanotube. Physical Review B, 2010, 81, .	3.2	5
85	Water-Induced Interactions between Boron-Doped Carbon Nanotubes. Journal of Physical Chemistry C, 2014, 118, 17838-17846.	3.1	5
86	Kinetic Monte Carlo Simulation of AC Impedance on the Cathode Side of a Solid Oxide Fuel Cell. Journal of the Electrochemical Society, 2010, 157, B90.	2.9	4
87	How Do Ionic Liquids â€œFoldâ€•Ionenes? Computational and Experimental Analysis of Imidazolium Polymers Based on Ether and Alkyl Chain Variations Dissolved in an Ionic Liquid. Macromolecules, 2021, 54, 1611-1622.	4.8	4
88	Molecular simulation of glycerol-derived triether podands for lithium ion solvation. Physical Chemistry Chemical Physics, 2022, 24, 9459-9466.	2.8	4
89	Tangible visualization of molecular dynamics simulations using 3-D printing. Education for Chemical Engineers, 2015, 13, 9-16.	4.8	3
90	Martini Coarse-Grained Model for Poly(alkylimidazolium) Ionenes and Applications in Aromatic Compound Extraction. Macromolecules, 2022, 55, 26-34.	4.8	3

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91	Atomistic Modeling of Solid Oxide Fuel Cells. Annual Reports in Computational Chemistry, 2010, , 201-234.	1.7	2
92	Understanding liquidâ€“liquid equilibria in binary mixtures of hydrocarbons with a thermally robust perarylphosphonium-based ionic liquid. RSC Advances, 2021, 11, 31328-31338.	3.6	2
93	Molecular simulations and experimental studies of the structural properties of imidazolium ionenes with butyl and decyl spacers solvated in 1-ethyl-3-methylimidazolium bistriflimide. Journal of Ionic Liquids, 2022, 2, 100013.	2.7	2
94	Tuning conformational structures of imidazolium ionenes with 1-ethyl-3-methylimidazolium ionic liquid solvents. Chemical Engineering Science, 2022, 251, 117456.	3.8	2
95	Quantifying the anion effect of gas solubility within ionic liquids using the solvation affinity index. Chemical Engineering Science, 2022, 260, 117851.	3.8	2
96	A COMBINED COMPUTATIONAL/EXPERIMENTAL STUDY OF FLUORESCENT GOLD NANOCLUSTER COMPLEXES. Nano LIFE, 2010, 01, 133-143.	0.9	1
97	Scalable, safer and greener syntheses of vinylimidazoles via reactive distillation of hydroxyethylimidazole intermediates. Polymer International, 2021, 70, 582-593.	3.1	1
98	Computational Catalysisâ€”Trends and Outlook. Catalysts, 2021, 11, 479.	3.5	0