# 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 | Molecular aspects of temperature swing solvent extraction for brine desalination using imidazole-based solvents. Chemical Engineering Science, 2022, 247, 116866. | 3.8 | 12 |
| 2 | Understanding gas absorption in multivalent ionic liquids via solute-solvent interaction analyses. Chemical Physics Letters, 2022, 786, 139204. | 2.6 | 7 |
| 3 | 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 |
| 4 | Tuning conformational structures of imidazolium ionenes with 1-ethyl-3-methylimidazolium ionic liquid solvents. Chemical Engineering Science, 2022, 251, 117456. | 3.8 | 2 |
| 5 | Charge scaling parameter evaluation for multivalent ionic liquids with fixed point charge force fields. Journal of Ionic Liquids, 2022, 2, 100020. | 2.7 | 8 |
| 6 | Molecular simulation of glycerol-derived triether podands for lithium ion solvation. Physical Chemistry Chemical Physics, 2022, 24, 9459-9466. | 2.8 | 4 |
| 7 | Martini Coarse-Grained Model for Poly(alkylimidazolium) Ionenes and Applications in Aromatic Compound Extraction. Macromolecules, 2022, 55, 26-34. | 4.8 | 3 |
| 8 | Computational and experimental study of different brines in temperature swing solvent extraction desalination with amine solvents. Desalination, 2022, 537, 115863. | 8.2 | 12 |
| 9 | Quantifying the anion effect of gas solubility within ionic liquids using the solvation affinity index. Chemical Engineering Science, 2022, 260, 117851. | 3.8 | 2 |
| 10 | Molecular-level behavior of imidazolium-based ionic liquid mixtures. Chemical Engineering Science, 2021, 229, 116073. | 3.8 | 16 |
| 11 | Scalable, safer and greener syntheses of vinylimidazoles via reactive distillation of hydroxyethylimidazole intermediates. Polymer International, 2021, 70, 582-593. | 3.1 | 1 |
| 12 | 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 |
| 13 | 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 |
| 14 | Computational Catalysisâ€”Trends and Outlook. Catalysts, 2021, 11, 479. | 3.5 | 0 |
| 15 | Screening Ionic Liquids Based on Ionic Volume and Electrostatic Potential Analyses. Journal of Physical Chemistry B, 2021, 125, 3653-3664. | 2.6 | 20 |
| 16 | Solubility Behavior of CO<sub>2</sub> in Ionic Liquids Based on Ionic Polarity Index Analyses. Journal of Physical Chemistry B, 2021, 125, 3665-3676. | 2.6 | 17 |
| 17 | Molecular Simulation of High-Salinity Brines in Contact with Diisopropylamine and Tripropylamine Solvents. Industrial & Engineering Chemistry Research, 2021, 60, 7917-7925. | 3.7 | 10 |
| 18 | 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 |

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|---|---|---|---|
| 19 | 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 |
| 20 | Computational study of the electrostatic potential and charges of multivalent ionic liquid molecules. Journal of Molecular Liquids, 2021, 340, 117190. | 4.9 | 9 |
| 21 | 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 |
| 22 | 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 |
| 23 | 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 |
| 24 | 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 |
| 25 | Molecular insight into the anion effect and free volume effect of CO<sub>2</sub>solubility in multivalent ionic liquids. Physical Chemistry Chemical Physics, 2020, 22, 20618-20633. | 2.8 | 27 |
| 26 | Properties of symmetric 1,3-diethers based on glycerol skeletons for CO2 absorption. Fluid Phase Equilibria, 2020, 521, 112718. | 2.5 | 11 |
| 27 | 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 |
| 28 | Structure and reactivity of single site Ti catalysts for propylene epoxidation. Journal of Catalysis, 2019, 377, 419-428. | 6.2 | 38 |
| 29 | Molecular Transport Behavior of CO<sub>2</sub> in Ionic Polyimides and Ionic Liquid Composite Membrane Materials. Journal of Physical Chemistry B, 2019, 123, 7455-7463. | 2.6 | 18 |
| 30 | 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 |
| 31 | 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 |
| 32 | 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 |
| 33 | Effects of TiO<sub>2</sub> in Low Temperature Propylene Epoxidation Using Gold Catalysts. Journal of Physical Chemistry C, 2018, 122, 1688-1698. | 3.1 | 37 |
| 34 | The Nitric Oxide Dimer Reaction in Carbon Nanopores. Journal of Physical Chemistry B, 2018, 122, 3604-3614. | 2.6 | 17 |
| 35 | 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 |
| 36 | Theoretical Studies on the Direct Propylene Epoxidation Using Gold-Based Catalysts: A Mini-Review. Catalysts, 2018, 8, 421. | 3.5 | 21 |

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| 37 | Mechanistic insights into the direct propylene epoxidation using Au nanoparticles dispersed on TiO2/SiO2. Chemical Engineering Science, 2018, 191, 169-182. | 3.8 | 26 |
| 38 | Analysis of the propylene epoxidation mechanism on supported gold nanoparticles. Chemical Engineering Science, 2017, 174, 229-237. | 3.8 | 20 |
| 39 | Confinement Effects on Carbon Dioxide Methanation: A Novel Mechanism for Abiotic Methane Formation. Scientific Reports, 2017, 7, 9021. | 3.3 | 31 |
| 40 | Molecular Simulation of Ionic Polyimides and Composites with Ionic Liquids as Gas-Separation Membranes. Langmuir, 2017, 33, 11377-11389. | 3.5 | 36 |
| 41 | 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 |
| 42 | 1,2,3-Trimethoxypropane: A Glycerol-Derived Physical Solvent for CO<sub>2</sub> Absorption. ACS Sustainable Chemistry and Engineering, 2017, 5, 911-921. | 6.7 | 28 |
| 43 | An Atomistic Carbide-Derived Carbon Model Generated Using ReaxFF-Based Quenched Molecular Dynamics. Journal of Carbon Research, 2017, 3, 32. | 2.7 | 13 |
| 44 | 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 |
| 45 | Modeling the atomistic growth behavior of gold nanoparticles in solution. Nanoscale, 2016, 8, 9354-9365. | 5.6 | 20 |
| 46 | Molecular Dynamics Simulation of Bismuth Telluride Exfoliation Mechanisms in Different Ionic Liquid Solvents. Langmuir, 2016, 32, 9982-9992. | 3.5 | 13 |
| 47 | Mechanism of Bismuth Telluride Exfoliation in an Ionic Liquid Solvent. Langmuir, 2015, 31, 3644-3652. | 3.5 | 45 |
| 48 | Tangible visualization of molecular dynamics simulations using 3-D printing. Education for Chemical Engineers, 2015, 13, 9-16. | 4.8 | 3 |
| 49 | 3D Printed Block Copolymer Nanostructures. Journal of Chemical Education, 2015, 92, 1866-1870. | 2.3 | 28 |
| 50 | Enhancing the pre-polymerization coordination of 1-vinylimidazole. Chemical Engineering Science, 2015, 138, 646-654. | 3.8 | 6 |
| 51 | Chemical and Physical Absorption of SO<sub>2</sub> by N-Functionalized Imidazoles: Experimental Results and Molecular-level Insight. Industrial & Engineering Chemistry Research, 2015, 54, 462-471. | 3.7 | 60 |
| 52 | Oxygen adsorption characteristics on hybrid carbon and boronâ€nitride nanotubes. Journal of Computational Chemistry, 2014, 35, 1058-1063. | 3.3 | 13 |
| 53 | Adsorption properties of nitrogen dioxide on hybrid carbon and boron-nitride nanotubes. Physical Chemistry Chemical Physics, 2014, 16, 22853-22860. | 2.8 | 31 |
| 54 | 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 |

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| 55 | Water-Induced Interactions between Boron-Doped Carbon Nanotubes. Journal of Physical Chemistry C, 2014, 118, 17838-17846. | 3.1 | 5 |
| 56 | 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 |
| 57 | 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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| 60 | 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 |
| 61 | 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 |
| 62 | Molecular Simulation of the Thermophysical Properties of N-Functionalized Alkylimidazoles. Journal of Physical Chemistry B, 2012, 116, 6529-6535. | 2.6 | 26 |
| 63 | Synthesis and Growth Mechanism of Iron Oxide Nanowhiskers. Nano Letters, 2011, 11, 1141-1146. | 9.1 | 92 |
| 64 | 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 |
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| 66 | 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 |
| 67 | Platinum attachments on iron oxide nanoparticle surfaces. Journal of Applied Physics, 2010, 107, 09B311. | 2.5 | 24 |
| 68 | A COMBINED COMPUTATIONAL/EXPERIMENTAL STUDY OF FLUORESCENT GOLD NANOCLUSTER COMPLEXES. Nano LIFE, 2010, 01, 133-143. | 0.9 | 1 |
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| 72 | Atomistic Modeling of Solid Oxide Fuel Cells. Annual Reports in Computational Chemistry, 2010, , 201-234. | 1.7 | 2 |

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| 73 | Molecular dynamics simulation of the Al<sub>2</sub>O<sub>3</sub>film structure during atomic layer deposition. Molecular Simulation, 2009, 35, 270-279. | 2.0 | 28 |
| 74 | First-principles study of methane dehydrogenation on a bimetallic Cu/Ni(111) surface. Journal of Chemical Physics, 2009, 131, 174702. | 3.0 | 94 |
| 75 | 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 |
| 76 | 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:m incorporation in the yttria stabilized zirconia (YSZ) fuel cell. Chemical Physics Letters, 2009, 471, 326-330. | 2.6 | 12 |
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| 78 | Transition-Metal Strings Templated on Boron-Doped Carbon Nanotubes: A DFT Investigation. Journal of Physical Chemistry C, 2009, 113, 15346-15354. | 3.1 | 12 |
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| 80 | Boron-doped carbon powders formed at 1000Â°C and one atmosphere. Carbon, 2008, 46, 1711-1717. | 10.3 | 59 |
| 81 | Simulation of chemical reaction equilibria by the reaction ensemble Monte Carlo method: a reviewâ€. Molecular Simulation, 2008, 34, 119-146. | 2.0 | 102 |
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| 91 | Adsorption and catalysis: The effect of confinement on chemical reactions. Applied Surface Science, 2005, 252, 766-777. | 6.1 | 85 |
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| 97 | Influence of chemical and physical surface heterogeneity on chemical reaction equilibria in carbon micropores. Molecular Physics, 2001, 99, 1991-2001. | 1.7 | 50 |
| 98 | Glycerolâ€derived Solvents Containing Two or Three Distinct Functional Groups Enabled by Trifluoroethyl Glycidyl Ether. AICHE Journal, 0, , e17533. | 3.6 | 8 |