

David C Cantu

List of Publications by Year in descending order

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33
papers

1,018
citations

516561

16
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434063

31
g-index

38
all docs

38
docs citations

38
times ranked

1227
citing authors

#	ARTICLE	IF	CITATIONS
1	Thioesterase enzyme families: Functions, structures, and mechanisms. <i>Protein Science</i> , 2022, 31, 652-676.	3.1	18
2	The solution structures and relative stability constants of lanthanide-EDTA complexes predicted from computation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 10263-10271.	1.3	4
3	Advanced Theory and Simulation to Guide the Development of CO ₂ Capture Solvents. <i>ACS Omega</i> , 2022, 7, 12453-12466.	1.6	2
4	Ionic Contraction across the Lanthanide Series Decreases the Temperature-Induced Disorder of the Water Coordination Sphere. <i>Inorganic Chemistry</i> , 2022, 61, 287-294.	1.9	10
5	Comparing conditional probabilities and statistical independence in layers of protection analysis. <i>Process Safety Progress</i> , 2021, 40, e12215.	0.4	2
6	Solution structure of a europium-nicotianamine complex supports that phytosiderophores bind lanthanides. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4287-4299.	1.3	12
7	Predicting lanthanide coordination structures in solution with molecular simulation. <i>Methods in Enzymology</i> , 2021, 651, 193-233.	0.4	3
8	Coordination Sphere of Lanthanide Aqua Ions Resolved with Ab Initio Molecular Dynamics and X-ray Absorption Spectroscopy. <i>Inorganic Chemistry</i> , 2021, 60, 3117-3130.	1.9	33
9	Norm-Conserving Pseudopotentials and Basis Sets to Explore Actinide Chemistry in Complex Environments. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3360-3371.	2.3	19
10	Effect of Lanthanum Ions on the Brønsted Acidity of Faujasite and Implications for Hydrothermal Stability. <i>Journal of Physical Chemistry C</i> , 2021, 125, 13649-13657.	1.5	10
11	Computational Prediction of All Lanthanide Aqua Ion Acidity Constants. <i>Inorganic Chemistry</i> , 2021, 60, 10257-10266.	1.9	9
12	On the Role of Enthalpic and Entropic Contributions to the Conformational Free Energy Landscape of MIL-101(Cr) Secondary Building Units. <i>Advanced Theory and Simulations</i> , 2020, 3, 2000092.	1.3	7
13	Subtle changes in hydrogen bond orientation result in glassification of carbon capture solvents. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19009-19021.	1.3	3
14	Molecular-Level Overhaul of Aminopropyl Aminosilicone/Triethylene Glycol Post-Combustion CO ₂ Capture Solvents. <i>ChemSusChem</i> , 2020, 13, 3429-3438.	3.6	16
15	Norm-Conserving Pseudopotentials and Basis Sets To Explore Lanthanide Chemistry in Complex Environments. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5987-5997.	2.3	46
16	Molecular Level Understanding of the Free Energy Landscape in Early Stages of Metal-Organic Framework Nucleation. <i>Journal of the American Chemical Society</i> , 2019, 141, 6073-6081.	6.6	23
17	Directed Hydrogen Bond Placement: Low Viscosity Amine Solvents for CO ₂ Capture. <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 7535-7542.	3.2	34
18	Water-Lean Solvents for Post-Combustion CO ₂ Capture: Fundamentals, Uncertainties, Opportunities, and Outlook. <i>Chemical Reviews</i> , 2017, 117, 9594-9624.	23.0	249

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19	Reinventing Design Principles for Developing Low-Viscosity Carbon Dioxide-Binding Organic Liquids for Flue Gas Clean Up. <i>ChemSusChem</i> , 2017, 10, 636-642.	3.6	26
20	Integrated Solvent Design for CO ₂ Capture and Viscosity Tuning. <i>Energy Procedia</i> , 2017, 114, 726-734.	1.8	10
21	Are Water-lean Solvent Systems Viable for Post-Combustion CO ₂ Capture?. <i>Energy Procedia</i> , 2017, 114, 756-763.	1.8	18
22	Structure-property reduced order model for viscosity prediction in single-component CO ₂ -binding organic liquids. <i>Green Chemistry</i> , 2016, 18, 6004-6011.	4.6	20
23	Dynamic Acid/Base Equilibrium in Single Component Switchable Ionic Liquids and Consequences on Viscosity. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1646-1652.	2.1	33
24	Molecular Mechanism of a Hotdog-Fold Acyl-CoA Thioesterase. <i>Chemistry - A European Journal</i> , 2014, 20, 9045-9051.	1.7	20
25	Formation Mechanism of the Secondary Building Unit in a Chromium Terephthalate Metal-Organic Framework. <i>Chemistry of Materials</i> , 2014, 26, 6401-6409.	3.2	33
26	Evaluating Transformational Solvent Systems for Post-combustion CO ₂ Separations. <i>Energy Procedia</i> , 2014, 63, 8144-8152.	1.8	15
27	Structural classification and properties of ketoacyl reductases, hydroxyacyl dehydratases and enoyl reductases. <i>Protein Engineering, Design and Selection</i> , 2012, 25, 803-811.	1.0	7
28	Acyl carrier protein structural classification and normal mode analysis. <i>Protein Science</i> , 2012, 21, 655-666.	3.1	11
29	Phylogenetic and experimental characterization of an acyl-ACP thioesterase family reveals significant diversity in enzymatic specificity and activity. <i>BMC Biochemistry</i> , 2011, 12, 44.	4.4	142
30	ThYme: a database for thioester-active enzymes. <i>Nucleic Acids Research</i> , 2011, 39, D342-D346.	6.5	55
31	Thioesterases: A new perspective based on their primary and tertiary structures. <i>Protein Science</i> , 2010, 19, 1281-1295.	3.1	121
32	Theory and computation show that Asp463 is the catalytic proton donor in human endoplasmic reticulum α -(1 \rightarrow 2)-mannosidase I. <i>Carbohydrate Research</i> , 2008, 343, 2235-2242.	1.1	6
33	Tailored Computational Approaches to Interrogate Heavy Element Chemistry and Structure in Condensed Phase. <i>ACS Symposium Series</i> , 0, , 219-245.	0.5	0