David C Cantu

List of Publications by Year
in descending order

33 papers	1,018 citations	516710 16 h-index	434195 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. Protein Science, 2022, 31, 652-676.	7.6	18
2	The solution structures and relative stability constants of lanthanideâ€“EDTA complexes predicted from computation. Physical Chemistry Chemical Physics, 2022, 24, 10263-10271.	2.8	4
3	Advanced Theory and Simulation to Guide the Development of CO₂ Capture Solvents. ACS Omega, 2022, 7, 12453-12466.	3.5	2
4	Ionic Contraction across the Lanthanide Series Decreases the Temperature-Induced Disorder of the Water Coordination Sphere. Inorganic Chemistry, 2022, 61, 287-294.	4.0	10
5	Comparing conditional probabilities and statistical independence in layers of protection analysis. Process Safety Progress, 2021, 40, e12215.	1.0	2
6	Solution structure of a europiumâ€“nicotianamine complex supports that phytosiderophores bind lanthanides. Physical Chemistry Chemical Physics, 2021, 23, 4287-4299.	2.8	12
7	Predicting lanthanide coordination structures in solution with molecular simulation. Methods in Enzymology, 2021, 651, 193-233.	1.0	3
8	Coordination Sphere of Lanthanide Aqua Ions Resolved with Ab Initio Molecular Dynamics and X-ray Absorption Spectroscopy. Inorganic Chemistry, 2021, 60, 3117-3130.	4.0	33
9	Norm-Conserving Pseudopotentials and Basis Sets to Explore Actinide Chemistry in Complex Environments. Journal of Chemical Theory and Computation, 2021, 17, 3360-3371.	5.3	19
10	Effect of Lanthanum Ions on the BrÃ¸nsted Acidity of Faujasite and Implications for Hydrothermal Stability. Journal of Physical Chemistry C, 2021, 125, 13649-13657.	3.1	10
11	Computational Prediction of All Lanthanide Aqua Ion Acidity Constants. Inorganic Chemistry, 2021, 60, 10257-10266.	4.0	9
12	On the Role of Enthalpic and Entropic Contributions to the Conformational Free Energy Landscape of MILâ€101(Cr) Secondary Building Units. Advanced Theory and Simulations, 2020, 3, 2000092.	2.8	7
13	Subtle changes in hydrogen bond orientation result in glassification of carbon capture solvents. Physical Chemistry Chemical Physics, 2020, 22, 19009-19021.	2.8	3
14	Molecularâ€Level Overhaul of Î³â€Aminopropyl Aminosilicone/Triethylene Glycol Postâ€Combustion CO₂â€Capture Solvents. ChemSusChem, 2020, 13, 3429-3438.	6.8	16
15	Norm-Conserving Pseudopotentials and Basis Sets To Explore Lanthanide Chemistry in Complex Environments. Journal of Chemical Theory and Computation, 2019, 15, 5987-5997.	5.3	46
16	Molecular Level Understanding of the Free Energy Landscape in Early Stages of Metalâ€“Organic Framework Nucleation. Journal of the American Chemical Society, 2019, 141, 6073-6081.	13.7	23
17	Directed Hydrogen Bond Placement: Low Viscosity Amine Solvents for CO₂ Capture. ACS Sustainable Chemistry and Engineering, 2019, 7, 7535-7542.	6.7	34
18	Water-Lean Solvents for Post-Combustion CO₂Capture: Fundamentals, Uncertainties, Opportunities, and Outlook. Chemical Reviews, 2017, 117, 9594-9624.	47.7	249

#	Article	IF	Citations
19	Reinventing Design Principles for Developing Lowâ€Viscosity Carbon Dioxideâ€Binding Organic Liquids for Flue Gas Clean Up. ChemSusChem, 2017, 10, 636-642.	6.8	26
20	Integrated Solvent Design for CO2 Capture and Viscosity Tuning. Energy Procedia, 2017, 114, 726-734.	1.8	10
21	Are Water-lean Solvent Systems Viable for Post-Combustion CO2 Capture?. Energy Procedia, 2017, 114, 756-763.	1.8	18
22	Structureâ€“property reduced order model for viscosity prediction in single-component CO₂-binding organic liquids. Green Chemistry, 2016, 18, 6004-6011.	9.0	20
23	Dynamic Acid/Base Equilibrium in Single Component Switchable Ionic Liquids and Consequences on Viscosity. Journal of Physical Chemistry Letters, 2016, 7, 1646-1652.	4.6	33
24	Molecular Mechanism of a Hotdogâ€Fold Acylâ€CoA Thioesterase. Chemistry - A European Journal, 2014, 20, 9045-9051.	3.3	20
25	Formation Mechanism of the Secondary Building Unit in a Chromium Terephthalate Metalâ€“Organic Framework. Chemistry of Materials, 2014, 26, 6401-6409.	6.7	33
26	Evaluating Transformational Solvent Systems for Post-combustion CO2 Separations. Energy Procedia, 2014, 63, 8144-8152.	1.8	15
27	Structural classification and properties of ketoacyl reductases, hydroxyacyl dehydratases and enoyl reductases. Protein Engineering, Design and Selection, 2012, 25, 803-811.	2.1	7
28	Acyl carrier protein structural classification and normal mode analysis. Protein Science, 2012, 21, 655-666.	7.6	11
29	Phylogenetic and experimental characterization of an acyl-ACP thioesterase family reveals significant diversity in enzymatic specificity and activity. BMC Biochemistry, 2011, 12, 44.	4.4	142
30	ThYme: a database for thioester-active enzymes. Nucleic Acids Research, 2011, 39, D342-D346.	14.5	55
31	Thioesterases: A new perspective based on their primary and tertiary structures. Protein Science, 2010, 19, 1281-1295.	7.6	121
32	Theory and computation show that Asp463 is the catalytic proton donor in human endoplasmic reticulum Î±-(1â†’2)-mannosidase I. Carbohydrate Research, 2008, 343, 2235-2242.	2.3	6
33	Tailored Computational Approaches to Interrogate Heavy Element Chemistry and Structure in Condensed Phase. ACS Symposium Series, 0, , 219-245.	0.5	0