

Santiago Aparicio

List of Publications by Year in descending order

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209
papers

7,420
citations

61984

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76900

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all docs

210
docs citations

210
times ranked

6008
citing authors

#	ARTICLE	IF	CITATIONS
1	A study on monoterpene-based natural deep eutectic solvents. <i>Green Chemical Engineering</i> , 2023, 4, 99-114.	6.3	7
2	On the behavior of quercetin in organic solvent solutions and their role for C60 fullerene solubilization. <i>Journal of Molecular Liquids</i> , 2022, 345, 117714.	4.9	2
3	Molecular dynamics study on the use of Deep Eutectic Solvents for Enhanced Oil Recovery. <i>Journal of Petroleum Science and Engineering</i> , 2022, 209, 109953.	4.2	15
4	Land Vulnerability, Risk Zoning, and Ecological Protection in the Protection Forest of Pagaibamba (Peru). <i>Forests</i> , 2022, 13, 436.	2.1	2
5	Insights on novel type V deep eutectic solvents based on levulinic acid. <i>Journal of Chemical Physics</i> , 2022, 156, 094504.	3.0	11
6	Molecular dynamics of CH_4 on calcite for enhancing gas recovery. <i>Canadian Journal of Chemical Engineering</i> , 2022, 100, 3184-3195.	1.7	2
7	Bulk liquid phase and interfacial behavior of cineole-based deep eutectic solvents with regard to carbon dioxide. <i>Journal of Molecular Liquids</i> , 2022, 353, 118748.	4.9	6
8	A theoretical study on CO_2 at Li_4SiO_4 and $\text{Li}_3\text{NaSiO}_4$ surfaces. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 13678-13689.	2.8	5
9	A density functional theory based tight-binding study on the water effect on nanostructuring of choline chloride + ethylene glycol deep eutectic solvent. <i>Journal of Chemical Physics</i> , 2022, 156, .	3.0	6
10	High-pressure carbon dioxide solubility in terpene based deep eutectic solvents. <i>Journal of Environmental Chemical Engineering</i> , 2022, 10, 108237.	6.7	14
11	A nanoscopic explanation of nitric oxide solubility in natural deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2021, 324, 114673.	4.9	7
12	CO ₂ enhanced gas recovery and sequestration in depleted gas reservoirs: A review. <i>Journal of Petroleum Science and Engineering</i> , 2021, 196, 107685.	4.2	125
13	Molecular insights into the production of few-layer graphene in N-Cyclohexylpyrrolidone + water mixtures. <i>Carbon</i> , 2021, 171, 723-738.	10.3	6
14	Effect of strain on gas adsorption in tight gas carbonates: A DFT study. <i>Computational Materials Science</i> , 2021, 188, 110186.	3.0	5
15	Theoretical studies of methane adsorption on Silica-Kaolinite interface for shale reservoir application. <i>Applied Surface Science</i> , 2021, 546, 149164.	6.1	23
16	Review and Perspectives for Effective Solutions to Grand Challenges of Energy and Fuels Technologies via Novel Deep Eutectic Solvents. <i>Energy & Fuels</i> , 2021, 35, 6402-6419.	5.1	46
17	Nanoscope characterization of type II porous liquid and its use for CO ₂ absorption from molecular simulation. <i>Journal of Molecular Liquids</i> , 2021, 330, 115660.	4.9	15
18	Theoretical insights into the cineole-based deep eutectic solvents. <i>Journal of Chemical Physics</i> , 2021, 154, 184504.	3.0	14

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19	Additivation of MoS ₂ nanosheets to synthetic poly-alpha-olefins base oils: A theoretical study of nanolubrication. <i>Journal of Molecular Liquids</i> , 2021, 332, 115881.	4.9	9
20	Experimental and molecular modeling study on the binary mixtures of [EMIM][BF ₄] and [EMIM][TFSI] ionic liquids. <i>Journal of Molecular Liquids</i> , 2021, 334, 116049.	4.9	14
21	A combined experimental and theoretical study on diglyme+1-alkanol liquid mixtures. <i>Journal of Molecular Liquids</i> , 2021, 334, 116048.	4.9	1
22	On the properties of N-methyl-2-pyrrolidonium hydrogen sulfate ionic liquid and alkanol mixtures. <i>Journal of Molecular Liquids</i> , 2021, 333, 115925.	4.9	2
23	The structure of CO ₂ and CH ₄ at the interface of a poly(urethane urea) oligomer model from the microscopic point of view. <i>Journal of Chemical Physics</i> , 2021, 155, 044704.	3.0	3
24	Low Toxicological Impact of Commercial Pristine Multi-Walled Carbon Nanotubes on the Yeast <i>Saccharomyces cerevisiae</i> . <i>Nanomaterials</i> , 2021, 11, 2272.	4.1	1
25	Molecular dynamics study on water confinement in deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2021, 339, 116758.	4.9	19
26	Ab-Initio Molecular Dynamics investigation of gas adsorption on α -quartz (001) for CO ₂ enhanced natural gas recovery. <i>Journal of Petroleum Science and Engineering</i> , 2021, 205, 108963.	4.2	2
27	Review on chemical enhanced oil recovery: Utilization of ionic liquids and deep eutectic solvents. <i>Journal of Petroleum Science and Engineering</i> , 2021, 205, 108746.	4.2	34
28	Influence of natural gas composition on adsorption in calcite Nanopores: A DFT study. <i>Applied Surface Science</i> , 2021, 568, 150940.	6.1	8
29	Insights on the water effect on deep eutectic solvents properties and structuring: The archetypical case of choline chloride+Ethylene glycol. <i>Journal of Molecular Liquids</i> , 2021, 344, 117717.	4.9	52
30	Nanosopic study on carvone-terpene based natural deep eutectic solvents. <i>Journal of Chemical Physics</i> , 2021, 155, 224702.	3.0	11
31	Nanostructuring and macroscopic behavior of type V deep eutectic solvents based on monoterpenoids. <i>Physical Chemistry Chemical Physics</i> , 2021, 24, 512-531.	2.8	28
32	A theoretical study of gas adsorption on calcite for CO ₂ enhanced natural gas recovery. <i>Applied Surface Science</i> , 2020, 504, 144575.	6.1	28
33	Quasi-smectic liquid crystal phase of octane in contact with 2D MoS ₂ . <i>Applied Surface Science</i> , 2020, 533, 147386.	6.1	5
34	Single atom transition metals on MoS ₂ monolayer and their use as catalysts for CO ₂ activation. <i>Applied Surface Science</i> , 2020, 534, 147611.	6.1	29
35	Insights into the interaction between lipid bilayers and trehalose aqueous solutions. <i>Journal of Molecular Liquids</i> , 2020, 314, 113639.	4.9	7
36	Behavior of Antibiotics in Natural Deep Eutectic Solvents. <i>Journal of Chemical & Engineering Data</i> , 2020, 65, 4669-4683.	1.9	9

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37	Ab Initio Molecular Dynamics Investigation of CH ₄ /CO ₂ Adsorption on Calcite: Improving the Enhanced Gas Recovery Process. ACS Omega, 2020, 5, 30226-30236.	3.5	6
38	Effect of Hydrogen Bond Donors and Acceptors on CO ₂ Absorption by Deep Eutectic Solvents. Processes, 2020, 8, 1533.	2.8	46
39	Long-Term Effects of the Application of Urban Waste Compost and Other Organic Amendments on Solanum tuberosum L.. Agronomy, 2020, 10, 1575.	3.0	7
40	Densification and tribofilm formation in hydrocarbon nanofluids induced by MoS ₂ nanotubes. Journal of Molecular Liquids, 2020, 311, 113291.	4.9	3
41	Insights on Betaine + Lactic Acid Deep Eutectic Solvent. Industrial & Engineering Chemistry Research, 2020, 59, 11880-11892.	3.7	21
42	Catalysis effect on CO ₂ methanation using MgH ₂ as a portable hydrogen medium. Physical Chemistry Chemical Physics, 2020, 22, 14720-14730.	2.8	7
43	Theoretical Study on Deep Eutectic Solvents as Vehicles for the Delivery of Anesthetics. Journal of Physical Chemistry B, 2020, 124, 1794-1805.	2.6	17
44	Ab Initio molecular dynamics of the dissolution of oilfield pyrite scale using borax. Journal of Molecular Liquids, 2020, 302, 112500.	4.9	15
45	Intermolecular forces in pyrrolidones + 1,2-alkanediol liquid mixtures. Journal of Molecular Liquids, 2020, 302, 112539.	4.9	2
46	Deep Eutectic Solvent Reline at 2D Nanomaterial Interfaces. Journal of Physical Chemistry B, 2020, 124, 1197-1206.	2.6	22
47	Effect of surface morphology on methane interaction with calcite: a DFT study. RSC Advances, 2020, 10, 16669-16674.	3.6	17
48	A theoretical study of gas adsorption on Î±-quartz (OÂÂ1) for CO ₂ enhanced natural gas recovery. Applied Surface Science, 2020, 525, 146472.	6.1	10
49	Insights on (C, BN, Si, Ge, MoS ₂) Nanotubes in Reline Deep Eutectic Solvent. Journal of Physical Chemistry B, 2020, 124, 3556-3567.	2.6	11
50	A Theoretical Study on Trehalose + Water Mixtures for Dry Preservation Purposes. Molecules, 2020, 25, 1435.	3.8	5
51	Quantum Chemistry Insight into the Interactions Between Deep Eutectic Solvents and SO ₂ . Molecules, 2019, 24, 2963.	3.8	36
52	An experimental study on doubly salt effect for methane hydrate inhibition. Journal of Natural Gas Science and Engineering, 2019, 72, 103015.	4.4	13
53	Effect of rock mineralogy on Hot-CO ₂ injection for enhanced gas recovery. Journal of Natural Gas Science and Engineering, 2019, 72, 103030.	4.4	19
54	Insights on [BMIM][BF ₄] and [BMIM][PF ₆] ionic liquids and their binary mixtures with acetone and acetonitrile. Journal of Molecular Liquids, 2019, 294, 111632.	4.9	13

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55	Theoretical Insights into CO ₂ Adsorption by MoS ₂ Nanomaterials. Journal of Physical Chemistry C, 2019, 123, 26338-26350.	3.1	18
56	An experimental and theoretical investigation of the physicochemical properties on choline chloride + Lactic acid based natural deep eutectic solvent (NADES). Journal of Molecular Liquids, 2019, 290, 110916.	4.9	57
57	Design of arginine-based therapeutic deep eutectic solvents as drug solubilization vehicles for active pharmaceutical ingredients. Physical Chemistry Chemical Physics, 2019, 21, 10621-10634.	2.8	54
58	Combined Experimental and Theoretical Study on High Pressure Methane Solubility in Natural Deep Eutectic Solvents. Industrial & Engineering Chemistry Research, 2019, 58, 8097-8111.	3.7	34
59	Molecular dynamics simulations of mixed deep eutectic solvents and their interaction with nanomaterials. Journal of Molecular Liquids, 2019, 283, 147-154.	4.9	43
60	Insights into Carbon Nanotubes and Fullerenes in Molten Alkali Carbonates. Journal of Physical Chemistry C, 2019, 123, 9909-9918.	3.1	3
61	Experimental and theoretical study of 2-hydroxyethylammonium formate ionic liquid + alcohol mixtures. Journal of Molecular Liquids, 2019, 281, 269-279.	4.9	13
62	A theoretical study on the adsorption of acid gases by boron nitride-based nanomaterials. Applied Surface Science, 2019, 480, 83-95.	6.1	13
63	A combined experimental and theoretical study on gas adsorption performance of amine and amide porous polymers. Microporous and Mesoporous Materials, 2019, 279, 61-72.	4.4	15
64	Intermolecular forces in 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide + ethanol mixtures. Journal of Molecular Liquids, 2018, 258, 1-9.	4.9	19
65	Gas solubility and rheological behavior study of betaine and alanine based natural deep eutectic solvents (NADES). Journal of Molecular Liquids, 2018, 256, 286-295.	4.9	76
66	Insights on the mixtures of imidazolium based ionic liquids with molecular solvents. Journal of Molecular Liquids, 2018, 255, 199-207.	4.9	30
67	Molecular Modeling Analysis of CO ₂ Absorption by Glymes. Journal of Physical Chemistry B, 2018, 122, 1948-1957.	2.6	4
68	Theoretical Study of Low Viscous Ionic Liquids at the Graphene Interface. Journal of Physical Chemistry C, 2018, 122, 1645-1656.	3.1	15
69	A theoretical study on mixtures of amino acid-based ionic liquids. Physical Chemistry Chemical Physics, 2018, 20, 10213-10223.	2.8	11
70	Microscopic characterization of mixtures of amino acid ionic liquids and organic solvents. Journal of Molecular Liquids, 2018, 250, 111-120.	4.9	8
71	Adsorption equilibrium studies of CO ₂ , CH ₄ and N ₂ on various modified zeolites at high pressures up to 200 bars. Microporous and Mesoporous Materials, 2018, 262, 49-58.	4.4	35
72	A nanoscopic approach on benzene-toluene-xylenes extraction by sulfolane. Journal of Molecular Liquids, 2018, 249, 1039-1046.	4.9	8

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73	Structural Elucidation of Covalent Organic Polymers (COP) and Their Linker Effect on Gas Adsorption Performance via Density Functional Theory Approach. <i>ChemistrySelect</i> , 2018, 3, 8294-8305.	1.5	6
74	A theoretical study on lidocaine solubility in deep eutectic solvents. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27464-27473.	2.8	54
75	Theoretical Study on Molten Alkali Carbonate Interfaces. <i>Langmuir</i> , 2018, 34, 13065-13076.	3.5	5
76	On the properties of (choline chloride+ lactac acid) deep eutectic solvent with methanol mixtures. <i>Journal of Molecular Liquids</i> , 2018, 272, 815-820.	4.9	49
77	Molecular Dynamics Simulations of Metal Nanoparticles in Deep Eutectic Solvents. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18029-18039.	3.1	19
78	Molecular dynamics and experimental characterization of [BMIM][BF ₄] and [BMIM][PF ₆] with ether cosolvent binary mixtures. <i>Journal of Molecular Liquids</i> , 2018, 271, 65-73.	4.9	8
79	Cost-effective alkylammonium formate-based protic ionic liquids for methane hydrate inhibition. <i>Journal of Natural Gas Science and Engineering</i> , 2018, 58, 59-68.	4.4	23
80	Theoretical Study of Oil Desulfuration by Ammonium-Based Deep Eutectic Solvents. <i>Energy & Fuels</i> , 2018, 32, 7497-7507.	5.1	20
81	Molecular Insights into Benzimidazole-Linked Polymer Interactions with Carbon Dioxide and Nitrogen. <i>ChemistrySelect</i> , 2018, 3, 3691-3701.	1.5	10
82	Simultaneous CO ₂ and SO ₂ capture by using ionic liquids: a theoretical approach. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5411-5422.	2.8	18
83	Rheological, Thermodynamic, and Gas Solubility Properties of Phenylacetic Acid-Based Deep Eutectic Solvents. <i>Chemical Engineering and Technology</i> , 2017, 40, 778-790.	1.5	35
84	Elucidating the Properties of Graphene-Deep Eutectic Solvents Interface. <i>Langmuir</i> , 2017, 33, 5154-5165.	3.5	42
85	Insights into Glycol Ether-Alkanol Mixtures from a Combined Experimental and Theoretical Approach. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5601-5612.	2.6	6
86	Investigation of the performance of biocompatible gas hydrate inhibitors via combined experimental and DFT methods. <i>Journal of Chemical Thermodynamics</i> , 2017, 111, 7-19.	2.0	20
87	Microscopic characterization of amino acid ionic liquids - water mixtures. <i>Journal of Molecular Liquids</i> , 2017, 236, 81-92.	4.9	10
88	Local environment structure and dynamics of CO ₂ in the 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide and related ionic liquids. <i>Journal of Chemical Physics</i> , 2017, 146, 104502.	3.0	8
89	Carbon Dioxide Solubility in Phosphonium-, Ammonium-, Sulfonyl-, and Pyrrolidinium-Based Ionic Liquids and their Mixtures at Moderate Pressures up to 10 bar. <i>Journal of Chemical & Engineering Data</i> , 2017, 62, 1310-1317.	1.9	25
90	High-pressure gas hydrate autoclave hydraulic experiments and scale-up modeling on the effect of stirring RPM effect. <i>Journal of Natural Gas Science and Engineering</i> , 2017, 38, 50-58.	4.4	46

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91	Behavior of Deep Eutectic Solvents under External Electric Fields: A Molecular Dynamics Approach. <i>Journal of Physical Chemistry B</i> , 2017, 121, 221-232.	2.6	21
92	On the behaviour of aqueous solutions of deep eutectic solvents at lipid biomembranes. <i>Journal of Molecular Liquids</i> , 2017, 247, 116-125.	4.9	22
93	Gas Solubility and Rheological Behavior of Natural Deep Eutectic Solvents (NADES) via Combined Experimental and Molecular Simulation Techniques. <i>ChemistrySelect</i> , 2017, 2, 7278-7295.	1.5	49
94	Gas hydrates inhibition via combined biomolecules and synergistic materials at wide process conditions. <i>Journal of Natural Gas Science and Engineering</i> , 2017, 46, 873-883.	4.4	53
95	Microscopic Characterization of CO ₂ and H ₂ S Removal by Sulfolane. <i>Energy & Fuels</i> , 2017, 31, 9800-9813.	5.1	8
96	A theoretical study on aminoacid-based ionic liquids with acid gases and water. <i>Journal of Molecular Liquids</i> , 2017, 225, 347-356.	4.9	10
97	High performance CO ₂ filtration and sequestration by using bromomethyl benzene linked microporous networks. <i>RSC Advances</i> , 2016, 6, 66324-66335.	3.6	6
98	Properties of Dialkylcarbonate + 1-Alkanol Mixtures at the Vacuum Interface. <i>Journal of Physical Chemistry C</i> , 2016, 120, 29126-29134.	3.1	3
99	Insights on 1-Butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide + Ethanol Liquid Mixtures: A Molecular Dynamics Approach. <i>Journal of Chemical & Engineering Data</i> , 2016, 61, 2729-2737.	1.9	14
100	High-Pressure Methane, Carbon Dioxide, and Nitrogen Adsorption on Amine-Impregnated Porous Montmorillonite Nanoclays. <i>Journal of Chemical & Engineering Data</i> , 2016, 61, 2749-2760.	1.9	38
101	Physicochemical Insights on Alkylcarbonate-Alkanol Solutions. <i>Journal of Physical Chemistry B</i> , 2016, 120, 5015-5028.	2.6	12
102	Investigation of Ester- and Amide-Linker-Based Porous Organic Polymers for Carbon Dioxide Capture and Separation at Wide Temperatures and Pressures. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 20772-20785.	8.0	52
103	Double Salt Ionic Liquids Based on Ammonium Cations and Their Application for CO ₂ Capture. <i>Journal of Physical Chemistry C</i> , 2016, 120, 17829-17844.	3.1	28
104	Insights into choline chloride-phenylacetic acid deep eutectic solvent for CO ₂ absorption. <i>RSC Advances</i> , 2016, 6, 109201-109210.	3.6	31
105	Interfacial properties of 1-ethyl-3-methylimidazolium glycinate ionic liquid regarding CO ₂ , SO ₂ and water from molecular dynamics. <i>Journal of Molecular Liquids</i> , 2016, 220, 910-917.	4.9	8
106	Deep Eutectic Solvents on the Surface of Face Centered Cubic Metals. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10400-10409.	3.1	29
107	Flavonol-carbon nanostructure hybrid systems: a DFT study on the interaction mechanism and UV/Vis features. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4760-4771.	2.8	7
108	A molecular dynamics study on aminoacid-based ionic liquids. <i>Journal of Molecular Liquids</i> , 2016, 213, 201-212.	4.9	33

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109	Experimental and DFT Approach on the Determination of Natural Gas Hydrate Equilibrium with the Use of Excess N ₂ and Choline Chloride Ionic Liquid as an Inhibitor. <i>Energy & Fuels</i> , 2016, 30, 2821-2832.	5.1	36
110	Synthesis, characterization and evaluation of porous polybenzimidazole materials for CO ₂ adsorption at high pressures. <i>Adsorption</i> , 2016, 22, 247-260.	3.0	15
111	Gas Hydrate Prevention and Flow Assurance by Using Mixtures of Ionic Liquids and Synergent Compounds: Combined Kinetics and Thermodynamic Approach. <i>Energy & Fuels</i> , 2016, 30, 3541-3548.	5.1	59
112	In silico rational design of ionic liquids for the exfoliation and dispersion of boron nitride nanosheets. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1212-1224.	2.8	20
113	A theoretical study on mitigation of CO ₂ through advanced deep eutectic solvents. <i>International Journal of Greenhouse Gas Control</i> , 2015, 39, 62-73.	4.6	55
114	Adsorption of choline benzoate ionic liquid on graphene, silicene, germanene and boron-nitride nanosheets: a DFT perspective. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16315-16326.	2.8	39
115	Interfacial Properties of Double Salt Ionic Liquids: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 28405-28416.	3.1	25
116	Thermodynamic characterization of deepwater natural gas mixtures with heavy hydrocarbon content at high pressures. <i>Journal of Chemical Thermodynamics</i> , 2015, 82, 134-142.	2.0	8
117	A detailed study of cholinium chloride and levulinic acid deep eutectic solvent system for CO ₂ capture via experimental and molecular simulation approaches. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 20941-20960.	2.8	133
118	Theoretical Study on the Solvation of C ₆₀ Fullerene by Ionic Liquids II: DFT Analysis of the Interaction Mechanism. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10616-10629.	2.6	9
119	An approach for the rationalization of melting temperature for deep eutectic solvents from DFT. <i>Chemical Physics Letters</i> , 2015, 634, 151-155.	2.6	111
120	Water Effect on Acid-Gas Capture Using Choline Lactate: A DFT Insight beyond Molecule-Molecule Pair Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 5546-5557.	2.6	14
121	A density functional theory insight towards the rational design of ionic liquids for SO ₂ capture. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 13559-13574.	2.8	37
122	Flavonols on graphene: a DFT insight. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	7
123	Deep Eutectic Solvents: Physicochemical Properties and Gas Separation Applications. <i>Energy & Fuels</i> , 2015, 29, 2616-2644.	5.1	777
124	Density Functional Theory Study on the Cholinium Dihydrogenphosphate Ionic Liquid for Acid Gas Removal. <i>Journal of Solution Chemistry</i> , 2015, 44, 890-899.	1.2	3
125	Characterization of Amide-Alkanediol Intermolecular Interactions. <i>Journal of Physical Chemistry B</i> , 2015, 119, 4725-4738.	2.6	13
126	Insights of CO ₂ adsorption performance of amine impregnated mesoporous silica (SBA-15) at wide range pressure and temperature conditions. <i>International Journal of Greenhouse Gas Control</i> , 2015, 43, 22-32.	4.6	44

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127	Nanowetting of Graphene by Ionic Liquid Droplets. Journal of Physical Chemistry C, 2015, 119, 24529-24537.	3.1	38
128	The impact of charges in force field parameterization for molecular dynamics simulations of deep eutectic solvents. Journal of Molecular Liquids, 2015, 211, 506-514.	4.9	69
129	Systematic Study on the Viscosity of Ionic Liquids: Measurement and Prediction. Industrial & Engineering Chemistry Research, 2015, 54, 10918-10924.	3.7	69
130	Theoretical Study of Renewable Ionic Liquids in the Pure State and with Graphene and Carbon Nanotubes. Journal of Physical Chemistry B, 2015, 119, 12224-12237.	2.6	15
131	Assessment of DFT methods for studying acid gas capture by ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 26875-26891.	2.8	27
132	Interaction Mechanism Insights on the Solvation of Fullerene C ₈₀ with Choline-based Ionic Liquids. Journal of Physical Chemistry B, 2015, 119, 12455-12463.	2.6	3
133	Interfacial Properties of Deep Eutectic Solvents Regarding to CO ₂ Capture. Journal of Physical Chemistry C, 2015, 119, 21413-21425.	3.1	81
134	Theoretical Study of Amino Acid-Based Ionic Liquids Interacting with Carbon Nanosystems. Journal of Physical Chemistry C, 2015, 119, 27080-27094.	3.1	21
135	Insights from quantum chemistry into piperazine-based ionic liquids and their behavior with regard to CO ₂ . Journal of Molecular Modeling, 2014, 20, 2107.	1.8	16
136	Theoretical Study on Amino Acid-Based Ionic Pairs and Their Interaction with Carbon Nanostructures. Journal of Physical Chemistry C, 2014, 118, 9741-9757.	3.1	34
137	Structure of Alkylcarbonate + <i>n</i> -Alkane Mixed Fluids. Journal of Physical Chemistry B, 2014, 118, 11310-11322.	2.6	11
138	Gas Hydrate Inhibition: A Review of the Role of Ionic Liquids. Industrial & Engineering Chemistry Research, 2014, 53, 17855-17868.	3.7	171
139	A theoretical study on ionic liquid endohedral C ₅₄₀ fullerene. RSC Advances, 2014, 4, 45286-45299.	3.6	3
140	Folding of Graphene Nanostructures Driven by Ionic Liquids Nanodroplets. Journal of Physical Chemistry C, 2014, 118, 21081-21091.	3.1	13
141	Insights into alkyl lactate+water mixed fluids. Journal of Molecular Liquids, 2014, 199, 215-223.	4.9	14
142	Theoretical Study on the Solvation of C ₆₀ Fullerene by Ionic Liquids. Journal of Physical Chemistry B, 2014, 118, 11330-11340.	2.6	25
143	Viscous origin of ionic liquids at the molecular level: A quantum chemical insight. Chemical Physics Letters, 2014, 610-611, 267-272.	2.6	7
144	A quantum chemistry study of natural gas hydrates. Journal of Molecular Modeling, 2014, 20, 2182.	1.8	18

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145	On the Properties of CO ₂ and Flue Gas at the Piperazinium-Based Ionic Liquids Interface: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 15061-15074.	3.1	22
146	Limitations and high pressure behavior of MOF-5 for CO ₂ capture. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14319.	2.8	42
147	Insights on cholinium- and piperazinium-based ionic liquids under external electric fields: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2013, 139, 224502.	3.0	12
148	Molecular Dynamics Study of Carbon Nanostructures in <i>N</i> -Methylpiperazinium Lactate Ionic Liquid. <i>Journal of Physical Chemistry C</i> , 2013, 117, 22046-22059.	3.1	21
149	Viscous Behavior of Imidazolium-Based Ionic Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2013, 52, 16774-16785.	3.7	64
150	High pressure CO ₂ absorption studies on imidazolium-based ionic liquids: Experimental and simulation approaches. <i>Fluid Phase Equilibria</i> , 2013, 351, 74-86.	2.5	56
151	P_{VT} measurements and derived properties of liquid 1,2-alkanediols. <i>Journal of Chemical Thermodynamics</i> , 2013, 57, 137-144.	2.0	29
152	A combined computational and experimental study of high pressure and supercritical CO ₂ adsorption on Basolite MOFs. <i>Microporous and Mesoporous Materials</i> , 2013, 175, 34-42.	4.4	45
153	Nanosopic Vision on Fuel Dearomatization Using Ionic Liquids: The Case of Piperazine-Based Fluids. <i>Energy & Fuels</i> , 2013, 27, 2515-2527.	5.1	22
154	Densities and Viscosities of Three Binary Monoglyme + 1-Alcohol Systems from (283.15 to 313.15) K. <i>Journal of Chemical & Engineering Data</i> , 2013, 58, 909-914.	1.9	35
155	Mixed Ionic Liquids: The Case of Pyridinium-Based Fluids. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2526-2537.	2.6	48
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