Santiago Aparicio

List of Publications by Year
in descending order

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209 papers	7,420 citations	61984 43 h-index	76900 74 g-index
210 all docs	210 docs citations	210 times ranked	6008 citing authors

#	Article	IF	Citations
1	Deep Eutectic Solvents: Physicochemical Properties and Gas Separation Applications. Energy & Fuels, 2015, 29, 2616-2644.	5.1	777
2	Review on the Use of Ionic Liquids (ILs) as Alternative Fluids for CO₂Capture and Natural Gas Sweetening. Energy & Fuels, 2010, 24, 5817-5828.	5.1	452
3	Thermophysical Properties of Pure Ionic Liquids: Review of Present Situation. Industrial & Engineering Chemistry Research, 2010, 49, 9580-9595.	3.7	395
4	The green solventethyl lactate: an experimental and theoretical characterization. Green Chemistry, 2009, 11, 65-78.	9.0	189
5	Gas Hydrate Inhibition: A Review of the Role of Ionic Liquids. Industrial & Engineering Chemistry Research, 2014, 53, 17855-17868.	3.7	171
6	Measurements and Modeling of Thermophysical Behavior of (C1â˜' C4) Alkylbenzoate/ (C1â˜' C11) Alkan-1-ol Mixed Solvents. Journal of Physical Chemistry B, 2004, 108, 15841-15850.	2.6	152
7	A detailed study of cholinium chloride and levulinic acid deep eutectic solvent system for CO₂ capture via experimental and molecular simulation approaches. Physical Chemistry Chemical Physics, 2015, 17, 20941-20960.	2.8	133
8	On the properties of 1-butyl-3-methylimidazolium octylsulfate ionic liquid. Green Chemistry, 2007, 9, 221-232.	9.0	130
9	CO2 enhanced gas recovery and sequestration in depleted gas reservoirs: A review. Journal of Petroleum Science and Engineering, 2021, 196, 107685.	4.2	125
10	An approach for the rationalization of melting temperature for deep eutectic solvents from DFT. Chemical Physics Letters, 2015, 634, 151-155.	2.6	111
11	Interfacial Properties of Deep Eutectic Solvents Regarding to CO₂ Capture. Journal of Physical Chemistry C, 2015, 119, 21413-21425.	3.1	81
12	The N-methylpyrrolidoneâ€"(C1â€"C10) alkan-1-ols solvent systemsElectronic Supplementary Information (ESI) available: Properties of pure components, densities, viscosities and refractive indices of mixtures NMP(1)â€‰+â€‰alkan-1-ols(2) at 298.15 K (Tables S1â€"S4). See http://www.rsc.org/suppdata/cp/b1/b109709c/. Physical Chemistry Chemical Physics, 2002, 4, 1170-1177.	2.8	78
13	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
14	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
15	Systematic Study on the Viscosity of Ionic Liquids: Measurement and Prediction. Industrial & Engineering Chemistry Research, 2015, 54, 10918-10924.	3.7	69
16	On the Viscosity of Pyridinium Based Ionic Liquids: An Experimental and Computational Study. Journal of Physical Chemistry B, 2011, 115, 12499-12513.	2.6	67
17	Thermophysical Behavior of Methylbenzoate + n-Alkanes Mixed Solvents. Application of Cubic Equations of State and Viscosity Models. Industrial & Engineering Chemistry Research, 2002, 41, 4399-4408.	3.7	66
18	A Systematic Computational Study on Flavonoids. International Journal of Molecular Sciences, 2010, 11, 2017-2038.	4.1	64

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19	Viscous Behavior of Imidazolium-Based Ionic Liquids. Industrial & Engineering Chemistry Research, 2013, 52, 16774-16785.	3.7	64
20	Gas Hydrate Prevention and Flow Assurance by Using Mixtures of Ionic Liquids and Synergent Compounds: Combined Kinetics and Thermodynamic Approach. Energy & Fuels, 2016, 30, 3541-3548.	5.1	59
21	An experimental and theoretical investigation of the physicochemical properties on choline chloride â€“ Lactic acid based natural deep eutectic solvent (NADES). Journal of Molecular Liquids, 2019, 290, 110916.	4.9	57
22	Thermophysical Behavior of n-Alkane + Alkylbenzoate Mixed Solvents. Measurements and Properties Modeling. Industrial & Engineering Chemistry Research, 2005, 44, 7575-7583.	3.7	56
23	High pressure CO2 absorption studies on imidazolium-based ionic liquids: Experimental and simulation approaches. Fluid Phase Equilibria, 2013, 351, 74-86.	2.5	56
24	Characterization of Lactam-Containing Binary Solvents by Solvatochromic Indicators. Journal of Physical Chemistry B, 2004, 108, 3024-3029.	2.6	55
25	Liquid structure of ethyl lactate, pure and water mixed, as seen by dielectric spectroscopy, solvatochromic and thermophysical studies. Chemical Physics Letters, 2008, 454, 49-55.	2.6	55
26	A Computational Study on Choline Benzoate and Choline Salicylate Ionic Liquids in the Pure State and After CO₂ Adsorption. Journal of Physical Chemistry B, 2012, 116, 9171-9185.	2.6	55
27	A theoretical study on mitigation of CO2 through advanced deep eutectic solvents. International Journal of Greenhouse Gas Control, 2015, 39, 62-73.	4.6	55
28	A theoretical study on lidocaine solubility in deep eutectic solvents. Physical Chemistry Chemical Physics, 2018, 20, 27464-27473.	2.8	54
29	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
30	Gas hydrates inhibition via combined biomolecules and synergistic materials at wide process conditions. Journal of Natural Gas Science and Engineering, 2017, 46, 873-883.	4.4	53
31	High-Pressure Study of the Methylsulfate and Tosylate Imidazolium Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 5593-5606.	2.6	52
32	Investigation of Ester- and Amide-Linker-Based Porous Organic Polymers for Carbon Dioxide Capture and Separation at Wide Temperatures and Pressures. ACS Applied Materials & Interfaces, 2016, 8, 20772-20785.	8.0	52
33	Insights on the water effect on deep eutectic solvents properties and structuring: The archetypical case of choline chlorideÂ+Âethylene glycol. Journal of Molecular Liquids, 2021, 344, 117717.	4.9	52
34	Choline-Based Ionic Liquids on Graphite Surfaces and Carbon Nanotubes Solvation: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2012, 116, 12055-12065.	3.1	50
35	PÏT measurements and derived properties of liquid 1-alkanols. Journal of Chemical Thermodynamics, 2012, 47, 241-259.	2.0	49
36	Gas Solubility and Rheological Behavior of Natural Deep Eutectic Solvents (NADES) via Combined Experimental and Molecular Simulation Techniques. ChemistrySelect, 2017, 2, 7278-7295.	1.5	49

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37	On the properties of (choline chlorideâ€¯+â€¯lactic acid) deep eutectic solvent with methanol mixtures. Journal of Molecular Liquids, 2018, 272, 815-820.	4.9	49
38	Mixed Ionic Liquids: The Case of Pyridinium-Based Fluids. Journal of Physical Chemistry B, 2012, 116, 2526-2537.	2.6	48
39	High-pressure gas hydrate autoclave hydraulic experiments and scale-up modeling on the effect of stirring RPM effect. Journal of Natural Gas Science and Engineering, 2017, 38, 50-58.	4.4	46
40	Effect of Hydrogen Bond Donors and Acceptors on CO2 Absorption by Deep Eutectic Solvents. Processes, 2020, 8, 1533.	2.8	46
41	Review and Perspectives for Effective Solutions to Grand Challenges of Energy and Fuels Technologies via Novel Deep Eutectic Solvents. Energy & Fuels, 2021, 35, 6402-6419.	5.1	46
42	Study on Hydroxylammonium-Based Ionic Liquids. I. Characterization. Journal of Physical Chemistry B, 2011, 115, 12473-12486.	2.6	45
43	A combined computational and experimental study of high pressure and supercritical CO2 adsorption on Basolite MOFs. Microporous and Mesoporous Materials, 2013, 175, 34-42.	4.4	45
44	Characterization of two lactones in liquid phase: an experimental and computational approach. Physical Chemistry Chemical Physics, 2009, 11, 6455.	2.8	44
45	Computational Study of Hexamethylguanidinium Lactate Ionic Liquid: A Candidate for Natural Gas Sweetening. Energy & Fuels, 2010, 24, 4989-5001.	5.1	44
46	Insights of CO2 adsorption performance of amine impregnated mesoporous silica (SBA-15) at wide range pressure and temperature conditions. International Journal of Greenhouse Gas Control, 2015, 43, 22-32.	4.6	44
47	Properties of 1,8-Cineole:â€‰ A Thermophysical and Theoretical Study. Journal of Physical Chemistry B, 2007, 111, 3167-3177.	2.6	43
48	CO₂ Adsorption Studies on Hydroxy Metal Carbonates M(CO₃)_x(OH)_y (M = Zn, Znâ€“Mg, Mg, Mgâ€“Cu, Cu, Ni,) Tj BT Q0 0 0 rgBT /Over	3.5	43
49	Molecular dynamics simulations of mixed deep eutectic solvents and their interaction with nanomaterials. Journal of Molecular Liquids, 2019, 283, 147-154.	4.9	43
50	Volumetric properties, viscosities and refractive indices of binary mixed solvents containing methyl benzoate. Physical Chemistry Chemical Physics, 2002, 4, 5833-5840.	2.8	42
51	Insights into the Ethyl Lactate + Water Mixed Solvent. Journal of Physical Chemistry B, 2009, 113, 14257-14269.	2.6	42
52	Limitations and high pressure behavior of MOF-5 for CO2 capture. Physical Chemistry Chemical Physics, 2013, 15, 14319.	2.8	42
53	Elucidating the Properties of Grapheneâ€“Deep Eutectic Solvents Interface. Langmuir, 2017, 33, 5154-5165.	3.5	42
54	Measurements and Predictive Models for the N-Methyl-2-pyrrolidone/Water/Methanol System. Journal of Physical Chemistry B, 2008, 112, 11361-11373.	2.6	40

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55	Adsorption of choline benzoate ionic liquid on graphene, silicene, germanene and boron-nitride nanosheets: a DFT perspective. Physical Chemistry Chemical Physics, 2015, 17, 16315-16326.	2.8	39
56	Nanowetting of Graphene by Ionic Liquid Droplets. Journal of Physical Chemistry C, 2015, 119, 24529-24537.	3.1	38
57	High-Pressure Methane, Carbon Dioxide, and Nitrogen Adsorption on Amine-Impregnated Porous Montmorillonite Nanoclays. Journal of Chemical & Engineering Data, 2016, 61, 2749-2760.	1.9	38
58	A density functional theory insight towards the rational design of ionic liquids for SO₂ capture. Physical Chemistry Chemical Physics, 2015, 17, 13559-13574.	2.8	37
59	Study on Hydroxylammonium-Based Ionic Liquids. II. Computational Analysis of CO₂Absorption. Journal of Physical Chemistry B, 2011, 115, 12487-12498.	2.6	36
60	Experimental and DFT Approach on the Determination of Natural Gas Hydrate Equilibrium with the Use of Excess N₂ and Choline Chloride Ionic Liquid as an Inhibitor. Energy & Fuels, 2016, 30, 2821-2832.	5.1	36
61	Quantum Chemistry Insight into the Interactions Between Deep Eutectic Solvents and SO2. Molecules, 2019, 24, 2963.	3.8	36
62	Densities and Viscosities of Three Binary Monoglyme + 1-Alcohol Systems from (283.15 to 313.15) K. Journal of Chemical & Engineering Data, 2013, 58, 909-914.	1.9	35
63	Rheological, Thermodynamic, and Gas Solubility Properties of Phenylacetic Acidâ€Based Deep Eutectic Solvents. Chemical Engineering and Technology, 2017, 40, 778-790.	1.5	35
64	Adsorption equilibrium studies of CO2, CH4 and N2 on various modified zeolites at high pressures up to 200 bars. Microporous and Mesoporous Materials, 2018, 262, 49-58.	4.4	35
65	Modeling the PVTx Behavior of the N-Methylpyrrolidinone/Water Mixed Solvent. Industrial & Engineering Chemistry Research, 2004, 43, 3205-3215.	3.7	34
66	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
67	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
68	Review on chemical enhanced oil recovery: Utilization of ionic liquids and deep eutectic solvents. Journal of Petroleum Science and Engineering, 2021, 205, 108746.	4.2	34
69	Pyrrolidone Derivatives in Water Solution: An Experimental and Theoretical Perspective. Industrial & Engineering Chemistry Research, 2009, 48, 1036-1050.	3.7	33
70	A molecular dynamics study on aminoacid-based ionic liquids. Journal of Molecular Liquids, 2016, 213, 201-212.	4.9	33
71	Viscosity Measurements and Data Correlation for Two Synthetic Natural Gas Mixtures. Journal of Chemical & Engineering Data, 2010, 55, 2498-2504.	1.9	31
72	Insights into choline chlorideâ€“phenylacetic acid deep eutectic solvent for CO₂ absorption. RSC Advances, 2016, 6, 109201-109210.	3.6	31

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73	Water effect on CO2 absorption for hydroxylammonium based ionic liquids: A molecular dynamics study. Chemical Physics, 2012, 400, 118-125.	1.9	30
74	Insights on the mixtures of imidazolium based ionic liquids with molecular solvents. Journal of Molecular Liquids, 2018, 255, 199-207.	4.9	30
75	Experimental and Computational Study on the Properties of Pure and Water Mixed 1-Ethyl-3-methylimidazolium l-(+)-Lactate Ionic Liquid. Journal of Physical Chemistry B, 2010, 114, 5795-5809.	2.6	29
76	PÏ measurements and derived properties of liquid 1,2-alkanediols. Journal of Chemical Thermodynamics, 2013, 57, 137-144.	2.0	29
77	Deep Eutectic Solvents on the Surface of Face Centered Cubic Metals. Journal of Physical Chemistry C, 2016, 120, 10400-10409.	3.1	29
78	Single atom transition metals on MoS2 monolayer and their use as catalysts for CO2 activation. Applied Surface Science, 2020, 534, 147611.	6.1	29
79	Double Salt Ionic Liquids Based on Ammonium Cations and Their Application for CO₂ Capture. Journal of Physical Chemistry C, 2016, 120, 17829-17844.	3.1	28
80	A theoretical study of gas adsorption on calcite for CO2 enhanced natural gas recovery. Applied Surface Science, 2020, 504, 144575.	6.1	28
81	Nanostructuring and macroscopic behavior of type V deep eutectic solvents based on monoterpenoids. Physical Chemistry Chemical Physics, 2021, 24, 512-531.	2.8	28
82	Soluteâ€“solvent interactions in the (N,N-dimethylformamide + N-methylformamide + water) ternary system at 298.15 K. Physical Chemistry Chemical Physics, 2001, 3, 2866-2871.	2.8	27
83	Thermophysical Properties of Binary and Ternary Mixtures Containing Lactams and Methanol. Industrial & Engineering Chemistry Research, 2009, 48, 10065-10076.	3.7	27
84	Assessment of DFT methods for studying acid gas capture by ionic liquids. Physical Chemistry Chemical Physics, 2015, 17, 26875-26891.	2.8	27
85	Theoretical Study on the Solvation of C60 Fullerene by Ionic Liquids. Journal of Physical Chemistry B, 2014, 118, 11330-11340.	2.6	25
86	Interfacial Properties of Double Salt Ionic Liquids: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2015, 119, 28405-28416.	3.1	25
87	Carbon Dioxide Solubility in Phosphonium-, Ammonium-, Sulfonyl-, and Pyrrolidinium-Based Ionic Liquids and their Mixtures at Moderate Pressures up to 10 bar. Journal of Chemical & Engineering Data, 2017, 62, 1310-1317.	1.9	25
88	Computational Study on the Properties and Structure of Methyl Lactate. Journal of Physical Chemistry A, 2007, 111, 4671-4683.	2.5	24
89	Study of Dimethoxyethane/Ethanol Solutions. Journal of Physical Chemistry B, 2011, 115, 8864-8874.	2.6	23
90	Cost-effective alkylammonium formate-based protic ionic liquids for methane hydrate inhibition. Journal of Natural Gas Science and Engineering, 2018, 58, 59-68.	4.4	23

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91	Theoretical studies of methane adsorption on Silica-Kaolinite interface for shale reservoir application. Applied Surface Science, 2021, 546, 149164.	6.1	23
92	On the Properties of CO₂ and Flue Gas at the Piperazinium-Based Ionic Liquids Interface: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2013, 117, 15061-15074.	3.1	22
93	Nanoscopic Vision on Fuel Dearomatization Using Ionic Liquids: The Case of Piperazine-Based Fluids. Energy & Fuels, 2013, 27, 2515-2527.	5.1	22
94	On the behaviour of aqueous solutions of deep eutectic solvents at lipid biomembranes. Journal of Molecular Liquids, 2017, 247, 116-125.	4.9	22
95	Deep Eutectic Solvent Reline at 2D Nanomaterial Interfaces. Journal of Physical Chemistry B, 2020, 124, 1197-1206.	2.6	22
96	Molecular Dynamics Study of Carbon Nanostructures in N-Methylpiperazinium Lactate Ionic Liquid. Journal of Physical Chemistry C, 2013, 117, 22046-22059.	3.1	21
97	Theoretical Study of Amino Acid-Based Ionic Liquids Interacting with Carbon Nanosystems. Journal of Physical Chemistry C, 2015, 119, 27080-27094.	3.1	21
98	Behavior of Deep Eutectic Solvents under External Electric Fields: A Molecular Dynamics Approach. Journal of Physical Chemistry B, 2017, 121, 221-232.	2.6	21
99	Insights on Betaine + Lactic Acid Deep Eutectic Solvent. Industrial & Engineering Chemistry Research, 2020, 59, 11880-11892.	3.7	21
100	In silico rational design of ionic liquids for the exfoliation and dispersion of boron nitride nanosheets. Physical Chemistry Chemical Physics, 2016, 18, 1212-1224.	2.8	20
101	Investigation of the performance of biocompatible gas hydrate inhibitors via combined experimental and DFT methods. Journal of Chemical Thermodynamics, 2017, 111, 7-19.	2.0	20
102	Theoretical Study of Oil Desulfuration by Ammonium-Based Deep Eutectic Solvents. Energy & Fuels, 2018, 32, 7497-7507.	5.1	20
103	Preferential Solvation in Ternary Solutions Containing Methylbenzoate. A Kirkwoodâ€'Buff Fluctuation Theory Study. Journal of Physical Chemistry B, 2003, 107, 13478-13486.	2.6	19
104	On the Viscosity of Natural Gases from Qatari North Field Reservoir. Journal of Chemical & Engineering Data, 2010, 55, 5117-5123.	1.9	19
105	pâ€"Ïâ€"TBehavior of Three Lean Synthetic Natural Gas Mixtures Using a Magnetic Suspension Densimeter and Isochoric Apparatus from (250 to 450) K with Pressures up to 150 MPa: Part II. Journal of Chemical & Engineering Data, 2011, 56, 3766-3774.	1.9	19
106	Intermolecular forces in 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide + ethanol mixtures. Journal of Molecular Liquids, 2018, 258, 1-9.	4.9	19
107	Molecular Dynamics Simulations of Metal Nanoparticles in Deep Eutectic Solvents. Journal of Physical Chemistry C, 2018, 122, 18029-18039.	3.1	19
108	Effect of rock mineralogy on Hot-CO2 injection for enhanced gas recovery. Journal of Natural Gas Science and Engineering, 2019, 72, 103030.	4.4	19

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109	Molecular dynamics study on water confinement in deep eutectic solvents. Journal of Molecular Liquids, 2021, 339, 116758.	4.9	19
110	Soluteâ€“solvent interactions in lactamsâ€“water ternary solvents. New Journal of Chemistry, 2005, 29, 817.	2.8	18
111	Microwave dielectric spectroscopy of 2-pyrrolidone+water mixtures. Chemical Physics Letters, 2007, 444, 252-257.	2.6	18
112	Isothermal PÏT measurements on Qatarâ€™s North Field type synthetic natural gas mixtures using a vibrating-tube densimeter. Journal of Chemical Thermodynamics, 2012, 53, 1-8.	2.0	18
113	A quantum chemistry study of natural gas hydrates. Journal of Molecular Modeling, 2014, 20, 2182.	1.8	18
114	Simultaneous CO₂ and SO₂ capture by using ionic liquids: a theoretical approach. Physical Chemistry Chemical Physics, 2017, 19, 5411-5422.	2.8	18
115	Theoretical Insights into CO₂ Adsorption by MoS₂ Nanomaterials. Journal of Physical Chemistry C, 2019, 123, 26338-26350.	3.1	18
116	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
117	Effect of surface morphology on methane interaction with calcite: a DFT study. RSC Advances, 2020, 10, 16669-16674.	3.6	17
118	PVTxMeasurements of theN-Methylpyrrolidone/Methanol Mixed Solvent:Â Cubic and SAFT EOS Analyses. Journal of Physical Chemistry B, 2006, 110, 6933-6942.	2.6	16
119	Insights from quantum chemistry into piperazine-based ionic liquids and their behavior with regard to CO2. Journal of Molecular Modeling, 2014, 20, 2107.	1.8	16
120	Thermophysical Behavior and Temperature Effect on the N-Methylpyrrolidone + (C1â^'C10) Alkan-1-ols Mixed Solvents. Industrial & Engineering Chemistry Research, 2003, 42, 920-928.	3.7	15
121	Liquidâ€“liquid equilibria of lactam containing binary systems. Fluid Phase Equilibria, 2008, 266, 90-100.	2.5	15
122	Insights into the Coal Extractive Solvent N-Methyl-2-pyrrolidone + Carbon Disulfide. Energy & Fuels, 2009, 23, 1591-1602.	5.1	15
123	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
124	Synthesis, characterization and evaluation of porous polybenzimidazole materials for CO2 adsorption at high pressures. Adsorption, 2016, 22, 247-260.	3.0	15
125	Theoretical Study of Low Viscous Ionic Liquids at the Graphene Interface. Journal of Physical Chemistry C, 2018, 122, 1645-1656.	3.1	15
126	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

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127	Ab Initio molecular dynamics of the dissolution of oilfield pyrite scale using borax. Journal of Molecular Liquids, 2020, 302, 112500.	4.9	15
128	Nanoscopic characterization of type II porous liquid and its use for CO2 absorption from molecular simulation. Journal of Molecular Liquids, 2021, 330, 115660.	4.9	15
129	Molecular dynamics study on the use of Deep Eutectic Solvents for Enhanced Oil Recovery. Journal of Petroleum Science and Engineering, 2022, 209, 109953.	4.2	15
130	Insights into alkyl lactate+water mixed fluids. Journal of Molecular Liquids, 2014, 199, 215-223.	4.9	14
131	Water Effect on Acid-Gas Capture Using Choline Lactate: A DFT Insight beyond Moleculeâ€“Molecule Pair Simulations. Journal of Physical Chemistry B, 2015, 119, 5546-5557.	2.6	14
132	Insights on 1-Butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide + Ethanol Liquid Mixtures: A Molecular Dynamics Approach. Journal of Chemical & Engineering Data, 2016, 61, 2729-2737.	1.9	14
133	Theoretical insights into the cineole-based deep eutectic solvents. Journal of Chemical Physics, 2021, 154, 184504.	3.0	14
134	Experimental and molecular modeling study on the binary mixtures of [EMIM][BF4] and [EMIM][TFSI] ionic liquids. Journal of Molecular Liquids, 2021, 334, 116049.	4.9	14
135	Natural Gas Hydrates. , 0, , .		14
136	High-pressure carbon dioxide solubility in terpene based deep eutectic solvents. Journal of Environmental Chemical Engineering, 2022, 10, 108237.	6.7	14
137	Folding of Graphene Nanostructures Driven by Ionic Liquids Nanodroplets. Journal of Physical Chemistry C, 2014, 118, 21081-21091.	3.1	13
138	Characterization of Amideâ€“Alkanediol Intermolecular Interactions. Journal of Physical Chemistry B, 2015, 119, 4725-4738.	2.6	13
139	An experimental study on doubly salt effect for methane hydrate inhibition. Journal of Natural Gas Science and Engineering, 2019, 72, 103015.	4.4	13
140	Insights on [BMIM][BF4] and [BMIM][PF6] ionic liquids and their binary mixtures with acetone and acetonitrile. Journal of Molecular Liquids, 2019, 294, 111632.	4.9	13
141	Experimental and theoretical study of 2-hydroxyethylammonium formate ionic liquid + alcohol mixtures. Journal of Molecular Liquids, 2019, 281, 269-279.	4.9	13
142	A theoretical study on the adsorption of acid gases by boron nitride-based nanomaterials. Applied Surface Science, 2019, 480, 83-95.	6.1	13
143	Structures of Alkyl Benzoate Binary Mixtures. A Kirkwoodâ€“Buff Fluctuation Theory Study Using UNIFAC. Journal of Physical Chemistry B, 2005, 109, 19908-19914.	2.6	12
144	Properties and Structure of Aromatic Ester Solvents. Journal of Physical Chemistry B, 2007, 111, 4417-4431.	2.6	12

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145	Insights on cholinium- and piperazinium-based ionic liquids under external electric fields: A molecular dynamics study. Journal of Chemical Physics, 2013, 139, 224502.	3.0	12
146	Physicochemical Insights on Alkylcarbonateâ€“Alkanol Solutions. Journal of Physical Chemistry B, 2016, 120, 5015-5028.	2.6	12
147	Structure of Alkylcarbonate + n-Alkane Mixed Fluids. Journal of Physical Chemistry B, 2014, 118, 11310-11322.	2.6	11
148	A theoretical study on mixtures of amino acid-based ionic liquids. Physical Chemistry Chemical Physics, 2018, 20, 10213-10223.	2.8	11
149	Insights on (C, BN, Si, Ge, MoS₂) Nanotubes in Reline Deep Eutectic Solvent. Journal of Physical Chemistry B, 2020, 124, 3556-3567.	2.6	11
150	Nanoscopic study on carvone-terpene based natural deep eutectic solvents. Journal of Chemical Physics, 2021, 155, 224702.	3.0	11
151	Insights on novel type V deep eutectic solvents based on levulinic acid. Journal of Chemical Physics, 2022, 156, 094504.	3.0	11
152	Microscopic characterization of amino acid ionic liquids - water mixtures. Journal of Molecular Liquids, 2017, 236, 81-92.	4.9	10
153	A theoretical study on aminoacid-based ionic liquids with acid gases and water. Journal of Molecular Liquids, 2017, 225, 347-356.	4.9	10
154	Molecular Insights into Benzimidazoleâ€Linked Polymer Interactions with Carbon Dioxide and Nitrogen. ChemistrySelect, 2018, 3, 3691-3701.	1.5	10
155	A theoretical study of gas adsorption on Î±-quartz (0Â0Â1) for CO2 enhanced natural gas recovery. Applied Surface Science, 2020, 525, 146472.	6.1	10
156	Microwave dielectric spectroscopy of pure and mixed aromatic ester solvents. PMC Physics B, 2008, 1, .	0.9	9
157	Optimized Binary Interaction Parameters for VLE Calculations of Natural Gas Mixtures via Cubic and Molecular-Based Equations of State. Industrial & Engineering Chemistry Research, 2012, 51, 9687-9699.	3.7	9
158	Theoretical Study on the Solvation of C₆₀ Fullerene by Ionic Liquids II: DFT Analysis of the Interaction Mechanism. Journal of Physical Chemistry B, 2015, 119, 10616-10629.	2.6	9
159	Behavior of Antibiotics in Natural Deep Eutectic Solvents. Journal of Chemical & Engineering Data, 2020, 65, 4669-4683.	1.9	9
160	Additivation of MoS2 nanosheets to synthetic poly-alpha-olefins base oils: A theoretical study of nanolubrication. Journal of Molecular Liquids, 2021, 332, 115881.	4.9	9
161	Compressed liquid density measurements for {methylbenzoate+(cyclohexane or 1-hexanol)} binary systems. Journal of Chemical Thermodynamics, 2011, 43, 1017-1022.	2.0	8
162	Thermodynamic characterization of deepwater natural gas mixtures with heavy hydrocarbon content at high pressures. Journal of Chemical Thermodynamics, 2015, 82, 134-142.	2.0	8

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163	Interfacial properties of 1-ethyl-3-methylimidazolium glycinate ionic liquid regarding CO2, SO2 and water from molecular dynamics. Journal of Molecular Liquids, 2016, 220, 910-917.	4.9	8
164	Local environment structure and dynamics of CO2 in the 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide and related ionic liquids. Journal of Chemical Physics, 2017, 146, 104502.	3.0	8
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