

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

139 papers	4,191 citations	31 h-index	58 g-index
141 ext. papers	4,798 ext. citations	4.1 avg, IF	6.13 L-index

#	Paper	IF	Citations
139	Deep Eutectic Solvents: Physicochemical Properties and Gas Separation Applications. <i>Energy & Fuels</i> , 2015 , 29, 2616-2644	4.1	575
138	Review on the Use of Ionic Liquids (ILs) as Alternative Fluids for CO ₂ Capture and Natural Gas Sweetening. <i>Energy & Fuels</i> , 2010 , 24, 5817-5828	4.1	396
137	Thermophysical Properties of Pure Ionic Liquids: Review of Present Situation. <i>Industrial & Engineering Chemistry Research</i> , 2010 , 49, 9580-9595	3.9	359
136	Gas Hydrate Inhibition: A Review of the Role of Ionic Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 17855-17868	3.9	139
135	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. <i>Coordination Chemistry Reviews</i> , 2015 , 304-305, 166-178	23.2	94
134	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, 20941-60	3.6	92
133	An approach for the rationalization of melting temperature for deep eutectic solvents from DFT. <i>Chemical Physics Letters</i> , 2015 , 634, 151-155	2.5	82
132	Interfacial Properties of Deep Eutectic Solvents Regarding to CO ₂ Capture. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 21413-21425	3.8	63
131	On the viscosity of pyridinium based ionic liquids: an experimental and computational study. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 12499-513	3.4	58
130	Two-electron versus one-electron reduction of chalcogens by uranium(III): synthesis of a terminal U(V) persulfide complex. <i>Chemical Science</i> , 2014 , 5, 841-846	9.4	54
129	Solution-based synthesis and processing of Sn- and Bi-doped Cu ₃ SbSe ₄ nanocrystals, nanomaterials and ring-shaped thermoelectric generators. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 2592-2602	13	53
128	Evaluating push-pull dye efficiency using TD-DFT and charge transfer indices. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 20210-9	3.6	53
127	Viscous Behavior of Imidazolium-Based Ionic Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2013 , 52, 16774-16785	3.9	52
126	A computational study on choline benzoate and choline salicylate ionic liquids in the pure state and after CO ₂ adsorption. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 9171-85	3.4	52
125	Systematic Study on the Viscosity of Ionic Liquids: Measurement and Prediction. <i>Industrial & Engineering Chemistry Research</i> , 2015 , 54, 10918-10924	3.9	51
124	The impact of charges in force field parameterization for molecular dynamics simulations of deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2015 , 211, 506-514	6	45
123	Choline-Based Ionic Liquids on Graphite Surfaces and Carbon Nanotubes Solvation: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 12055-12065	3.8	44

122	Ionic liquid design for enhanced carbon dioxide capture by computer-aided molecular design approach. <i>Clean Technologies and Environmental Policy</i> , 2015 , 17, 1301-1312	4.3	43
121	Gas solubility and rheological behavior study of betaine and alanine based natural deep eutectic solvents (NADES). <i>Journal of Molecular Liquids</i> , 2018 , 256, 286-295	6	42
120	Theoretical Study of the Effect of Alkyl and Alkoxy Lateral Chains on the Structural and Electronic Properties of π -Conjugated Polymers Consisting of Phenylethynyl-1,3,4-thiadiazole. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 2865-2873	3.8	42
119	Study on hydroxylammonium-based ionic liquids. I. Characterization. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 12473-86	3.4	42
118	Computational Study of Hexamethylguanidinium Lactate Ionic Liquid: A Candidate for Natural Gas Sweetening. <i>Energy & Fuels</i> , 2010 , 24, 4989-5001	4.1	41
117	CO ₂ adsorption studies on hydroxy metal carbonates M(CO ₃) _x (OH) _y (M = Zn, Zn-Mg, Mg, Mg-Cu, Cu, Ni, and Pb) at high pressures up to 175 bar. <i>Langmuir</i> , 2011 , 27, 10642-7	4	38
116	A comprehensive review on the rheological behavior of imidazolium based ionic liquids and natural deep eutectic solvents. <i>Journal of Molecular Liquids</i> , 2019 , 277, 932-958	6	38
115	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	4.2	35
114	Study on hydroxylammonium-based ionic liquids. II. Computational analysis of CO ₂ absorption. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 12487-98	3.4	34
113	Nanowetting of Graphene by Ionic Liquid Droplets. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 24529-24538	3.8	33
112	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	1.8	32
111	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, 16315-26	3.6	32
110	An experimental and theoretical investigation of the physicochemical properties on choline chloride-L-lactic acid based natural deep eutectic solvent (NADES). <i>Journal of Molecular Liquids</i> , 2019 , 290, 110916	6	31
109	A density functional theory insight towards the rational design of ionic liquids for SO ₂ capture. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 13559-74	3.6	31
108	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	4.6	31
107	Elucidating the Properties of Graphene-Deep Eutectic Solvents Interface. <i>Langmuir</i> , 2017 , 33, 5154-5165	4	30
106	Molecular dynamics simulations of mixed deep eutectic solvents and their interaction with nanomaterials. <i>Journal of Molecular Liquids</i> , 2019 , 283, 147-154	6	30
105	A molecular dynamics study on aminoacid-based ionic liquids. <i>Journal of Molecular Liquids</i> , 2016 , 213, 201-212	6	30

104	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	4.1	30
103	Theoretical Study on Amino Acid-Based Ionic Pairs and Their Interaction with Carbon Nanostructures. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 9741-9757	3.8	30
102	On the properties of (choline chloride + lactic acid) deep eutectic solvent with methanol mixtures. <i>Journal of Molecular Liquids</i> , 2018 , 272, 815-820	6	30
101	Optoelectronic and Charge Transport Properties of Oligomers Based on Phenylethynylene Units Linked to Thieno-acenes: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 6922-6932	3.8	29
100	Experimental and computational study on the properties of pure and water mixed 1-ethyl-3-methylimidazolium L-(+)-lactate ionic liquid. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 5795-8004	3.4	28
99	Theoretical study of the effect of ethynyl group on the structure and electrical properties of phenyl-thiadiazole systems as precursors of electron-conducting materials. <i>Journal of Chemical Physics</i> , 2009 , 130, 234907	3.9	28
98	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	3.8	26
97	Insights into choline chloride-phenylacetic acid deep eutectic solvent for CO ₂ absorption. <i>RSC Advances</i> , 2016 , 6, 109201-109210	3.7	26
96	Water effect on CO ₂ absorption for hydroxylammonium based ionic liquids: A molecular dynamics study. <i>Chemical Physics</i> , 2012 , 400, 118-125	2.3	26
95	Density functional theory study of the optical and electronic properties of oligomers based on phenyl-ethynyl units linked to triazole, thiadiazole, and oxadiazole rings to be used in molecular electronics. <i>Journal of Chemical Physics</i> , 2010 , 132, 064901	3.9	26
94	Rheological, Thermodynamic, and Gas Solubility Properties of Phenylacetic Acid-Based Deep Eutectic Solvents. <i>Chemical Engineering and Technology</i> , 2017 , 40, 778-790	2	24
93	Combined Experimental and Theoretical Study on High Pressure Methane Solubility in Natural Deep Eutectic Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 8097-8111	3.9	23
92	Assessment of DFT methods for studying acid gas capture by ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 26875-91	3.6	22
91	Effect of Hydrogen Bond Donors and Acceptors on CO ₂ Absorption by Deep Eutectic Solvents. <i>Processes</i> , 2020 , 8, 1533	2.9	22
90	Deep Eutectic Solvents on the Surface of Face Centered Cubic Metals. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 10400-10409	3.8	22
89	Interfacial Properties of Double Salt Ionic Liquids: A Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 28405-28416	3.8	22
88	Nanosopic Vision on Fuel Dearomatization Using Ionic Liquids: The Case of Piperazine-Based Fluids. <i>Energy & Fuels</i> , 2013 , 27, 2515-2527	4.1	22
87	Confinement Effects on UV-Visible Absorption Spectra: β -Carotene Inside Carbon Nanotube as a Test Case. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 1239-43	6.4	22

86	Theoretical study on the solvation of C60 fullerene by ionic liquids. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 11330-40	3.4	21
85	Corrosion Behavior of Carbon Steel in CO2 Saturated Amine and Imidazolium-, Ammonium-, and Phosphonium-Based Ionic Liquid Solutions. <i>Industrial & Engineering Chemistry Research</i> , 2016 , 55, 446-454	3.9	20
84	On the Properties of CO2 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	3.8	20
83	Molecular Dynamics Study of Carbon Nanostructures in N-Methylpiperazinium Lactate Ionic Liquid. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 22046-22059	3.8	20
82	Poly(arylenethynyl-thienoacenes) as candidates for organic semiconducting materials. A DFT insight. <i>Organic Electronics</i> , 2012 , 13, 3244-3253	3.5	20
81	Force Transmission Error Analysis for a High-Pressure Single-Sinker Magnetic Suspension Densimeter. <i>International Journal of Thermophysics</i> , 2010 , 31, 698-709	2.1	20
80	Behavior of Deep Eutectic Solvents under External Electric Fields: A Molecular Dynamics Approach. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 221-232	3.4	19
79	Theoretical Study of Amino Acid-Based Ionic Liquids Interacting with Carbon Nanosystems. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 27080-27094	3.8	19
78	DFT Study of the Ambipolar Character of Polymers on the Basis of s-Tetrazine and Aryl Rings. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 4588-4599	3.8	19
77	Thermoelectric Properties of Doped-CuSbSe Compounds: A First-Principles Insight. <i>Inorganic Chemistry</i> , 2018 , 57, 7321-7333	5.1	19
76	Theoretical Study of Bis(phenylethynyl)thienoacenes as Precursors of Molecular Wires for Molecular Electronics. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 12325-12334	3.8	18
75	Simultaneous CO and SO capture by using ionic liquids: a theoretical approach. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 5411-5422	3.6	17
74	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	2.8	17
73	On the behaviour of aqueous solutions of deep eutectic solvents at lipid biomembranes. <i>Journal of Molecular Liquids</i> , 2017 , 247, 116-125	6	17
72	Quantum Chemistry Insight into the Interactions Between Deep Eutectic Solvents and SO. <i>Molecules</i> , 2019 , 24,	4.8	17
71	In silico rational design of ionic liquids for the exfoliation and dispersion of boron nitride nanosheets. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 1212-24	3.6	16
70	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	4.6	16
69	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	2.9	15

68	Insights from quantum chemistry into piperazine-based ionic liquids and their behavior with regard to CO ₂ . <i>Journal of Molecular Modeling</i> , 2014 , 20, 2107	2	15
67	Theoretical estimation of the optical bandgap in a series of poly(aryl-ethynylene)s: a DFT study. <i>Journal of Chemical Physics</i> , 2014 , 140, 044908	3.9	15
66	Theoretical Study of Oil Desulfuration by Ammonium-Based Deep Eutectic Solvents. <i>Energy & Fuels</i> , 2018 , 32, 7497-7507	4.1	14
65	Electronic properties of diphenyl-s-tetrazine and some related oligomers. An spectroscopic and theoretical study. <i>Chemical Physics</i> , 2012 , 408, 17-27	2.3	14
64	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	4.1	14
63	Intermolecular forces in 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide + ethanol mixtures. <i>Journal of Molecular Liquids</i> , 2018 , 258, 1-9	6	13
62	Influence of chromium hyperdoping on the electronic structure of CH ₃ NH ₃ PbI ₃ perovskite: a first-principles insight. <i>Scientific Reports</i> , 2018 , 8, 2511	4.9	13
61	Electronic Structure and Charge Transport Properties of a Series of 3,6-(Diphenyl)-s-tetrazine Derivatives: Are They Suitable Candidates for Molecular Electronics?. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 26427-26439	3.8	13
60	Folding of Graphene Nanostructures Driven by Ionic Liquids Nanodroplets. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 21081-21091	3.8	13
59	Insights into alkyl lactate + water mixed fluids. <i>Journal of Molecular Liquids</i> , 2014 , 199, 215-223	6	13
58	A quantum chemistry study of natural gas hydrates. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2182	2	13
57	Crystal structure and charge transport properties of poly(arylene-ethynylene) derivatives: a DFT approach. <i>Journal of Chemical Physics</i> , 2013 , 138, 154902	3.9	13
56	DFT study of the effect of fluorine atoms on the crystal structure and semiconducting properties of poly(arylene-ethynylene) derivatives. <i>Journal of Chemical Physics</i> , 2016 , 144, 154902	3.9	13
55	Characterization of amide-alkanediol intermolecular interactions. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 4725-38	3.4	12
54	Theoretical Study of Renewable Ionic Liquids in the Pure State and with Graphene and Carbon Nanotubes. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 12224-37	3.4	12
53	Deep Eutectic Solvent Reline at 2D Nanomaterial Interfaces. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 1197-1206	3.4	12
52	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	4.4	12
51	A DFT approach to the charge transport related properties in columnar stacked π -conjugated N-heterocycle cores including electron donor and acceptor units. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 605-18	3.6	11

50	Physicochemical Insights on Alkylcarbonate-Alkanol Solutions. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 5015-28	3.4	11
49	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, 5546-57	3.4	10
48	A theoretical study on mixtures of amino acid-based ionic liquids. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 10213-10223	3.6	10
47	Molecular Insights into Benzimidazole-Linked Polymer Interactions with Carbon Dioxide and Nitrogen. <i>ChemistrySelect</i> , 2018 , 3, 3691-3701	1.8	10
46	Structure of alkylcarbonate + n-alkane mixed fluids. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 11310-223.4	3.4	10
45	Influence of the alkyl and alkoxy side chains on the electronic structure and charge-transport properties of polythiophene derivatives. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 10091-9	3.6	10
44	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	6	10
43	Insights on Betaine + Lactic Acid Deep Eutectic Solvent. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 11880-11892	3.9	9
42	An experimental study on doubly salt effect for methane hydrate inhibition. <i>Journal of Natural Gas Science and Engineering</i> , 2019 , 72, 103015	4.6	9
41	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	3.9	9
40	Theoretical Approach to the Study of Thiophene-Based Discotic Systems As Organic Semiconductors. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 15-22	3.8	9
39	A theoretical study on aminoacid-based ionic liquids with acid gases and water. <i>Journal of Molecular Liquids</i> , 2017 , 225, 347-356	6	9
38	A Tuned LRC-DFT Design of Ambipolar Diketopyrrolopyrrole-Containing Quinoidal Molecules Interesting for Molecular Electronics. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2591-601	6.4	9
37	Permeabilities of CO, HS and CH through Choline-Based Ionic Liquids: Atomistic-Scale Simulations. <i>Molecules</i> , 2019 , 24,	4.8	8
36	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	6	8
35	Viscous origin of ionic liquids at the molecular level: A quantum chemical insight. <i>Chemical Physics Letters</i> , 2014 , 610-611, 267-272	2.5	7
34	Microscopic characterization of mixtures of amino acid ionic liquids and organic solvents. <i>Journal of Molecular Liquids</i> , 2018 , 250, 111-120	6	7
33	Microscopic characterization of amino acid ionic liquids - water mixtures. <i>Journal of Molecular Liquids</i> , 2017 , 236, 81-92	6	6

32	Vanadium supersaturated silicon system: a theoretical and experimental approach. <i>Journal Physics D: Applied Physics</i> , 2017 , 50, 495101	3	6
31	Theoretical Study on the Solvation of C60 Fullerene by Ionic Liquids II: DFT Analysis of the Interaction Mechanism. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 10616-29	3-4	6
30	Flavonol-carbon nanostructure hybrid systems: a DFT study on the interaction mechanism and UV/Vis features. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 4760-71	3.6	6
29	Does the number of nitrogen atoms have an influence on the conducting properties of diphenylazines? A DFT insight. <i>Chemical Physics</i> , 2011 , 379, 51-56	2.3	6
28	The Role of Linear Alkyl and Alkoxy Side Chains in the Modulation of the Structure and Electrical Properties of Bithiophene: a Theoretical Study. <i>Australian Journal of Chemistry</i> , 2010 , 63, 1297	1.2	6
27	Insights into Glycol Ether-Alkanol Mixtures from a Combined Experimental and Theoretical Approach. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 5601-5612	3-4	5
26	Insights on (C, BN, Si, Ge, MoS) Nanotubes in Reline Deep Eutectic Solvent. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 3556-3567	3-4	5
25	Microscopic Characterization of CO ₂ and H ₂ S Removal by Sulfolane. <i>Energy & Fuels</i> , 2017 , 31, 9800-9813	3-4	5
24	First principle study of V-implantation in highly-doped silicon materials. <i>Computational Materials Science</i> , 2017 , 136, 207-215	3.2	5
23	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	1.8	5
22	Flavonols on graphene: a DFT insight. <i>Theoretical Chemistry Accounts</i> , 2015 , 134, 1	1.9	4
21	Transition Metal-Hyperdoped InP Semiconductors as Efficient Solar Absorber Materials. <i>Nanomaterials</i> , 2020 , 10,	5-4	4
20	Molecular Modeling Analysis of CO Absorption by Glymes. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 1948-1957	3-4	4
19	Spinel-Type nitride compounds with improved features as solar cell absorbers. <i>Acta Materialia</i> , 2020 , 197, 316-329	8.4	4
18	Effect of five-membered ring and heteroatom substitution on charge transport properties of perylene discotic derivatives: A theoretical approach. <i>Journal of Chemical Physics</i> , 2016 , 145, 054903	3-9	4
17	Density Functional Theory Study on the Cholinium Dihydrogenphosphate Ionic Liquid for Acid Gas Removal. <i>Journal of Solution Chemistry</i> , 2015 , 44, 890-899	1.8	3
16	Interaction Mechanism Insights on the Solvation of Fullerene B(80) with Choline-based Ionic Liquids. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 12455-63	3-4	3
15	Band Alignment of the CuGaS Chalcopyrite Interfaces Studied by First-Principles Calculations. <i>ACS Omega</i> , 2020 , 5, 3294-3301	3-9	3

14	A theoretical study on ionic liquid endohedral C540 fullerene. <i>RSC Advances</i> , 2014 , 4, 45286-45299	3.7	3
13	Molecular structure, conformational preferences and vibrational analysis of 2-hydroxystyrene: A computational and spectroscopic research. <i>Chemical Physics</i> , 2010 , 374, 62-76	2.3	3
12	Theoretical insights into the cineole-based deep eutectic solvents. <i>Journal of Chemical Physics</i> , 2021 , 154, 184504	3.9	3
11	Properties of Dialkylcarbonate + 1-Alkanol Mixtures at the Vacuum Interface. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 29126-29134	3.8	3
10	Nanostructuring and macroscopic behavior of type V deep eutectic solvents based on monoterpenoids.. <i>Physical Chemistry Chemical Physics</i> , 2021 , 24, 512-531	3.6	2
9	Molecular dynamics study on the use of Deep Eutectic Solvents for Enhanced Oil Recovery. <i>Journal of Petroleum Science and Engineering</i> , 2021 , 209, 109953	4.4	2
8	The effects of the chemical composition on the structural, thermodynamic, and mechanical properties of all-inorganic halide perovskites. <i>Inorganic Chemistry Frontiers</i> , 2021 , 8, 3803-3814	6.8	2
7	Thermoradiative Cells Based on a p-type Cu3SbSe4 Semiconductor: Application of a Detailed Balance Model. <i>Journal of Electronic Materials</i> , 2019 , 48, 6777-6785	1.9	1
6	Applications of Ionic Liquids in Gas Processing 2012 , 133-138		1
5	Nanosopic study on carvone-terpene based natural deep eutectic solvents.. <i>Journal of Chemical Physics</i> , 2021 , 155, 224702	3.9	1
4	Insights on novel type V deep eutectic solvents based on levulinic acid.. <i>Journal of Chemical Physics</i> , 2022 , 156, 094504	3.9	1
3	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	6	1
2	On the behavior of quercetin + organic solvent solutions and their role for C60 fullerene solubilization. <i>Journal of Molecular Liquids</i> , 2022 , 345, 117714	6	0
1	Cation substitution effects on the structural, electronic and sun-light absorption features of all-inorganic halide perovskites. <i>Inorganic Chemistry Frontiers</i> , 2022 , 9, 1337-1353	6.8	0