Gregorio Garca

List of Publications by Year in Descending Order

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	On the behavior of quercetin + organic solvent solutions and their role for C60 fullerene solubilization. *Journal of Molecular Liquids*, **2022**, 345, 117714	6	0
138	Cation substitution effects on the structural, electronic and sun-light absorption features of all-inorganic halide perovskites. *Inorganic Chemistry Frontiers*, **2022**, 9, 1337-1353	6.8	0
137	Insights on novel type V deep eutectic solvents based on levulinic acid.. *Journal of Chemical Physics*, **2022**, 156, 094504	3.9	1
136	Bulk liquid phase and interfacial behavior of cineole Based deep eutectic solvents with regard to carbon dioxide. *Journal of Molecular Liquids*, **2022**, 353, 118748	6	1
135	Nanostructuring and macroscopic behavior of type V deep eutectic solvents based on monoterpenoids.. *Physical Chemistry Chemical Physics*, **2021**, 24, 512-531	3.6	2
134	Nanoscopic study on carvone-terpene based natural deep eutectic solvents.. *Journal of Chemical Physics*, **2021**, 155, 224702	3.9	1
133	Molecular dynamics study on the use of Deep Eutectic Solvents for Enhanced Oil Recovery. *Journal of Petroleum Science and Engineering*, **2021**, 209, 109953	4.4	2
132	Insights on the water effect on deep eutectic solvents properties and structuring: The archetypical case of choline chloride+ethylene glycol. *Journal of Molecular Liquids*, **2021**, 344, 117717	6	10
131	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	4.1	14
130	Theoretical insights into the cineole-based deep eutectic solvents. *Journal of Chemical Physics*, **2021**, 154, 184504	3.9	3
129	The effects of the chemical composition on the structural, thermodynamic, and mechanical properties of all-inorganic halide perovskites. *Inorganic Chemistry Frontiers*, **2021**, 8, 3803-3814	6.8	2
128	Review on chemical enhanced oil recovery: Utilization of ionic liquids and deep eutectic solvents. *Journal of Petroleum Science and Engineering*, **2021**, 205, 108746	4.4	12
127	Effect of Hydrogen Bond Donors and Acceptors on CO2 Absorption by Deep Eutectic Solvents. *Processes*, **2020**, 8, 1533	2.9	22
126	Insights on Betaine + Lactic Acid Deep Eutectic Solvent. *Industrial & Engineering Chemistry Research*, **2020**, 59, 11880-11892	3.9	9
125	Band Alignment of the CuGaS Chalcopyrite Interfaces Studied by First-Principles Calculations. *ACS Omega*, **2020**, 5, 3294-3301	3.9	3
124	Transition Metal-Hyperdoped InP Semiconductors as Efficient Solar Absorber Materials. *Nanomaterials*, **2020**, 10,	5.4	4
123	Deep Eutectic Solvent Reline at 2D Nanomaterial Interfaces. *Journal of Physical Chemistry B*, **2020**, 124, 1197-1206	3.4	12

122	Insights on (C, BN, Si, Ge, MoS) Nanotubes in Reline Deep Eutectic Solvent. *Journal of Physical Chemistry B*, **2020**, 124, 3556-3567	3.4	5
121	Spinel-Type nitride compounds with improved features as solar cell absorbers. *Acta Materialia*, **2020**, 197, 316-329	8.4	4
120	Permeabilities of CO, HS and CH through Choline-Based Ionic Liquids: Atomistic-Scale Simulations. *Molecules*, **2019**, 24,	4.8	8
119	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	6	31
118	Combined Experimental and Theoretical Study on High Pressure Methane Solubility in Natural Deep Eutectic Solvents. *Industrial & Engineering Chemistry Research*, **2019**, 58, 8097-8111	3.9	23
117	Molecular dynamics simulations of mixed deep eutectic solvents and their interaction with nanomaterials. *Journal of Molecular Liquids*, **2019**, 283, 147-154	6	30
116	Quantum Chemistry Insight into the Interactions Between Deep Eutectic Solvents and SO. *Molecules*, **2019**, 24,	4.8	17
115	Thermoradiative Cells Based on a p-type Cu3SbSe4 Semiconductor: Application of a Detailed Balance Model. *Journal of Electronic Materials*, **2019**, 48, 6777-6785	1.9	1
114	An experimental study on doubly salt effect for methane hydrate inhibition. *Journal of Natural Gas Science and Engineering*, **2019**, 72, 103015	4.6	9
113	A comprehensive review on the rheological behavior of imidazolium based ionic liquids and natural deep eutectic solvents. *Journal of Molecular Liquids*, **2019**, 277, 932-958	6	38
112	Intermolecular forces in 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide + ethanol mixtures. *Journal of Molecular Liquids*, **2018**, 258, 1-9	6	13
111	Gas solubility and rheological behavior study of betaine and alanine based natural deep eutectic solvents (NADES). *Journal of Molecular Liquids*, **2018**, 256, 286-295	6	42
110	Molecular Modeling Analysis of CO Absorption by Glymes. *Journal of Physical Chemistry B*, **2018**, 122, 1948-1957	3.4	4
109	Influence of chromium hyperdoping on the electronic structure of CHNHPbI perovskite: a first-principles insight. *Scientific Reports*, **2018**, 8, 2511	4.9	13
108	A theoretical study on mixtures of amino acid-based ionic liquids. *Physical Chemistry Chemical Physics*, **2018**, 20, 10213-10223	3.6	10
107	Cost-effective alkylammonium formate-based protic ionic liquids for methane hydrate inhibition. *Journal of Natural Gas Science and Engineering*, **2018**, 58, 59-68	4.6	16
106	Theoretical Study of Oil Desulfuration by Ammonium-Based Deep Eutectic Solvents. *Energy & Fuels*, **2018**, 32, 7497-7507	4.1	14
105	Molecular Insights into Benzimidazole-Linked Polymer Interactions with Carbon Dioxide and Nitrogen. *ChemistrySelect*, **2018**, 3, 3691-3701	1.8	10

104	Microscopic characterization of mixtures of amino acid ionic liquids and organic solvents. *Journal of Molecular Liquids*, **2018**, 250, 111-120	6	7
103	Structural Elucidation of Covalent Organic Polymers (COP) and Their Linker Effect on Gas Adsorption Performance via Density Functional Theory Approach. *ChemistrySelect*, **2018**, 3, 8294-8305	1.8	5
102	On the properties of (choline chloride + lactic acid) deep eutectic solvent with methanol mixtures. *Journal of Molecular Liquids*, **2018**, 272, 815-820	6	30
101	Thermoelectric Properties of Doped-CuSbSe Compounds: A First-Principles Insight. *Inorganic Chemistry*, **2018**, 57, 7321-7333	5.1	19
100	Simultaneous CO and SO capture by using ionic liquids: a theoretical approach. *Physical Chemistry Chemical Physics*, **2017**, 19, 5411-5422	3.6	17
99	Rheological, Thermodynamic, and Gas Solubility Properties of Phenylacetic Acid-Based Deep Eutectic Solvents. *Chemical Engineering and Technology*, **2017**, 40, 778-790	2	24
98	Elucidating the Properties of Graphene-Deep Eutectic Solvents Interface. *Langmuir*, **2017**, 33, 5154-5165	4	30
97	Insights into Glycol Ether-Alkanol Mixtures from a Combined Experimental and Theoretical Approach. *Journal of Physical Chemistry B*, **2017**, 121, 5601-5612	3.4	5
96	Investigation of the performance of biocompatible gas hydrate inhibitors via combined experimental and DFT methods. *Journal of Chemical Thermodynamics*, **2017**, 111, 7-19	2.9	15
95	Microscopic characterization of amino acid ionic liquids - water mixtures. *Journal of Molecular Liquids*, **2017**, 236, 81-92	6	6
94	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	2.8	17
93	Behavior of Deep Eutectic Solvents under External Electric Fields: A Molecular Dynamics Approach. *Journal of Physical Chemistry B*, **2017**, 121, 221-232	3.4	19
92	Solution-based synthesis and processing of Sn- and Bi-doped Cu3SbSe4 nanocrystals, nanomaterials and ring-shaped thermoelectric generators. *Journal of Materials Chemistry A*, **2017**, 5, 2592-2602	13	53
91	On the behaviour of aqueous solutions of deep eutectic solvents at lipid biomembranes. *Journal of Molecular Liquids*, **2017**, 247, 116-125	6	17
90	Vanadium supersaturated silicon system: a theoretical and experimental approach. *Journal Physics D: Applied Physics*, **2017**, 50, 495101	3	6
89	Gas Solubility and Rheological Behavior of Natural Deep Eutectic Solvents (NADES) via Combined Experimental and Molecular Simulation Techniques. *ChemistrySelect*, **2017**, 2, 7278-7295	1.8	32
88	Gas hydrates inhibition via combined biomolecules and synergistic materials at wide process conditions. *Journal of Natural Gas Science and Engineering*, **2017**, 46, 873-883	4.6	31
87	Microscopic Characterization of CO2and H2S Removal by Sulfolane. *Energy & Fuels*, **2017**, 31, 9800-9813	3	5

86	A theoretical study on aminoacid-based ionic liquids with acid gases and water. *Journal of Molecular Liquids*, **2017**, 225, 347-356	6	9
85	First principle study of V-implantation in highly-doped silicon materials. *Computational Materials Science*, **2017**, 136, 207-215	3.2	5
84	Double Salt Ionic Liquids Based on Ammonium Cations and Their Application for CO2 Capture. *Journal of Physical Chemistry C*, **2016**, 120, 17829-17844	3.8	26
83	Insights into choline chloride–phenylacetic acid deep eutectic solvent for CO2 absorption. *RSC Advances*, **2016**, 6, 109201-109210	3.7	26
82	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	6	8
81	Deep Eutectic Solvents on the Surface of Face Centered Cubic Metals. *Journal of Physical Chemistry C*, **2016**, 120, 10400-10409	3.8	22
80	Flavonol-carbon nanostructure hybrid systems: a DFT study on the interaction mechanism and UV/Vis features. *Physical Chemistry Chemical Physics*, **2016**, 18, 4760-71	3.6	6
79	A molecular dynamics study on aminoacid-based ionic liquids. *Journal of Molecular Liquids*, **2016**, 213, 201-212	6	30
78	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	4.1	30
77	Corrosion Behavior of Carbon Steel in CO2 Saturated Amine and Imidazolium-, Ammonium-, and Phosphonium-Based Ionic Liquid Solutions. *Industrial & Engineering Chemistry Research*, **2016**, 55, 446-454	3.9	20
76	In silico rational design of ionic liquids for the exfoliation and dispersion of boron nitride nanosheets. *Physical Chemistry Chemical Physics*, **2016**, 18, 1212-24	3.6	16
75	Effect of five-membered ring and heteroatom substitution on charge transport properties of perylene discotic derivatives: A theoretical approach. *Journal of Chemical Physics*, **2016**, 145, 054903	3.9	4
74	Properties of Dialkylcarbonate + 1-Alkanol Mixtures at the Vacuum Interface. *Journal of Physical Chemistry C*, **2016**, 120, 29126-29134	3.8	3
73	DFT study of the effect of fluorine atoms on the crystal structure and semiconducting properties of poly(arylene-ethynylene) derivatives. *Journal of Chemical Physics*, **2016**, 144, 154902	3.9	13
72	Physicochemical Insights on Alkylcarbonate-Alkanol Solutions. *Journal of Physical Chemistry B*, **2016**, 120, 5015-28	3.4	11
71	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, 20941-60	3.6	92
70	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, 10616-29	3.4	6
69	An approach for the rationalization of melting temperature for deep eutectic solvents from DFT. *Chemical Physics Letters*, **2015**, 634, 151-155	2.5	82

68	Water Effect on Acid-Gas Capture Using Choline Lactate: A DFT Insight beyond Molecule-Molecule Pair Simulations. *Journal of Physical Chemistry B*, **2015**, 119, 5546-57	3.4	10
67	A density functional theory insight towards the rational design of ionic liquids for SO2 capture. *Physical Chemistry Chemical Physics*, **2015**, 17, 13559-74	3.6	31
66	Exploring excited states using Time Dependent Density Functional Theory and density-based indexes. *Coordination Chemistry Reviews*, **2015**, 304-305, 166-178	23.2	94
65	Flavonols on graphene: a DFT insight. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	4
64	Ionic liquid design for enhanced carbon dioxide capture by computer-aided molecular design approach. *Clean Technologies and Environmental Policy*, **2015**, 17, 1301-1312	4.3	43
63	Deep Eutectic Solvents: Physicochemical Properties and Gas Separation Applications. *Energy & Fuels*, **2015**, 29, 2616-2644	4.1	575
62	Density Functional Theory Study on the Cholinium Dihydrogenphosphate Ionic Liquid for Acid Gas Removal. *Journal of Solution Chemistry*, **2015**, 44, 890-899	1.8	3
61	Characterization of amide-alkanediol intermolecular interactions. *Journal of Physical Chemistry B*, **2015**, 119, 4725-38	3.4	12
60	Nanowetting of Graphene by Ionic Liquid Droplets. *Journal of Physical Chemistry C*, **2015**, 119, 24529-24537	4.8	33
59	The impact of charges in force field parameterization for molecular dynamics simulations of deep eutectic solvents. *Journal of Molecular Liquids*, **2015**, 211, 506-514	6	45
58	Systematic Study on the Viscosity of Ionic Liquids: Measurement and Prediction. *Industrial & Engineering Chemistry Research*, **2015**, 54, 10918-10924	3.9	51
57	Theoretical Study of Renewable Ionic Liquids in the Pure State and with Graphene and Carbon Nanotubes. *Journal of Physical Chemistry B*, **2015**, 119, 12224-37	3.4	12
56	Assessment of DFT methods for studying acid gas capture by ionic liquids. *Physical Chemistry Chemical Physics*, **2015**, 17, 26875-91	3.6	22
55	Interaction Mechanism Insights on the Solvation of Fullerene B(80)with Choline-based Ionic Liquids. *Journal of Physical Chemistry B*, **2015**, 119, 12455-63	3.4	3
54	Interfacial Properties of Deep Eutectic Solvents Regarding to CO2 Capture. *Journal of Physical Chemistry C*, **2015**, 119, 21413-21425	3.8	63
53	Theoretical Study of Amino Acid-Based Ionic Liquids Interacting with Carbon Nanosystems. *Journal of Physical Chemistry C*, **2015**, 119, 27080-27094	3.8	19
52	A DFT approach to the charge transport related properties in columnar stacked Π-conjugated N-heterocycle cores including electron donor and acceptor units. *Physical Chemistry Chemical Physics*, **2015**, 17, 605-18	3.6	11
51	A theoretical study on mitigation of CO2 through advanced deep eutectic solvents. *International Journal of Greenhouse Gas Control*, **2015**, 39, 62-73	4.2	35

50	Adsorption of choline benzoate ionic liquid on graphene, silicene, germanene and boron-nitride nanosheets: a DFT perspective. *Physical Chemistry Chemical Physics*, **2015**, 17, 16315-26	3.6	32
49	Interfacial Properties of Double Salt Ionic Liquids: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2015**, 119, 28405-28416	3.8	22
48	DFT Study of the Ambipolar Character of Polymers on the Basis of s-Tetrazine and Aryl Rings. *Journal of Physical Chemistry C*, **2015**, 119, 4588-4599	3.8	19
47	Insights from quantum chemistry into piperazine-based ionic liquids and their behavior with regard to CO *Journal of Molecular Modeling*, **2014**, 20, 2107	2	15
46	Theoretical Study on Amino Acid-Based Ionic Pairs and Their Interaction with Carbon Nanostructures. *Journal of Physical Chemistry C*, **2014**, 118, 9741-9757	3.8	30
45	Electronic Structure and Charge Transport Properties of a Series of 3,6-(Diphenyl)-s-tetrazine Derivatives: Are They Suitable Candidates for Molecular Electronics?. *Journal of Physical Chemistry C*, **2014**, 118, 26427-26439	3.8	13
44	Two-electron versus one-electron reduction of chalcogens by uranium(III): synthesis of a terminal U(V) persulfide complex. *Chemical Science*, **2014**, 5, 841-846	9.4	54
43	Structure of alkylcarbonate + n-alkane mixed fluids. *Journal of Physical Chemistry B*, **2014**, 118, 11310-22	3.4	10
42	Theoretical estimation of the optical bandgap in a series of poly(aryl-ethynylene)s: a DFT study. *Journal of Chemical Physics*, **2014**, 140, 044908	3.9	15
41	Gas Hydrate Inhibition: A Review of the Role of Ionic Liquids. *Industrial & Engineering Chemistry Research*, **2014**, 53, 17855-17868	3.9	139
40	A theoretical study on ionic liquid endohedral C540 fullerene. *RSC Advances*, **2014**, 4, 45286-45299	3.7	3
39	Folding of Graphene Nanostructures Driven by Ionic Liquids Nanodroplets. *Journal of Physical Chemistry C*, **2014**, 118, 21081-21091	3.8	13
38	Insights into alkyl lactate + water mixed fluids. *Journal of Molecular Liquids*, **2014**, 199, 215-223	6	13
37	Theoretical study on the solvation of C60 fullerene by ionic liquids. *Journal of Physical Chemistry B*, **2014**, 118, 11330-40	3.4	21
36	Viscous origin of ionic liquids at the molecular level: A quantum chemical insight. *Chemical Physics Letters*, **2014**, 610-611, 267-272	2.5	7
35	A quantum chemistry study of natural gas hydrates. *Journal of Molecular Modeling*, **2014**, 20, 2182	2	13
34	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	3.8	20
33	Insights on cholinium- and piperazinium-based ionic liquids under external electric fields: a molecular dynamics study. *Journal of Chemical Physics*, **2013**, 139, 224502	3.9	9

32	Evaluating push-pull dye efficiency using TD-DFT and charge transfer indices. *Physical Chemistry Chemical Physics*, **2013**, 15, 20210-9	3.6	53
31	Crystal structure and charge transport properties of poly(arylene-ethynylene) derivatives: a DFT approach. *Journal of Chemical Physics*, **2013**, 138, 154902	3.9	13
30	Molecular Dynamics Study of Carbon Nanostructures in N-Methylpiperazinium Lactate Ionic Liquid. *Journal of Physical Chemistry C*, **2013**, 117, 22046-22059	3.8	20
29	Viscous Behavior of Imidazolium-Based Ionic Liquids. *Industrial & Engineering Chemistry Research*, **2013**, 52, 16774-16785	3.9	52
28	Theoretical Approach to the Study of Thiophene-Based Discotic Systems As Organic Semiconductors. *Journal of Physical Chemistry C*, **2013**, 117, 15-22	3.8	9
27	Nanoscopic Vision on Fuel Dearomatization Using Ionic Liquids: The Case of Piperazine-Based Fluids. *Energy & Fuels*, **2013**, 27, 2515-2527	4.1	22
26	A Tuned LRC-DFT Design of Ambipolar Diketopyrrolopyrrole-Containing Quinoidal Molecules Interesting for Molecular Electronics. *Journal of Chemical Theory and Computation*, **2013**, 9, 2591-601	6.4	9
25	Confinement Effects on UV-Visible Absorption Spectra: Carotene Inside Carbon Nanotube as a Test Case. *Journal of Physical Chemistry Letters*, **2013**, 4, 1239-43	6.4	22
24	Electronic properties of diphenyl-s-tetrazine and some related oligomers. An spectroscopic and theoretical study. *Chemical Physics*, **2012**, 408, 17-27	2.3	14
23	Choline-Based Ionic Liquids on Graphite Surfaces and Carbon Nanotubes Solvation: A Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2012**, 116, 12055-12065	3.8	44
22	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, 9171-85	3.4	52
21	Poly(arylenethynyl-thienoacenes) as candidates for organic semiconducting materials. A DFT insight. *Organic Electronics*, **2012**, 13, 3244-3253	3.5	20
20	Water effect on CO2 absorption for hydroxylammonium based ionic liquids: A molecular dynamics study. *Chemical Physics*, **2012**, 400, 118-125	2.3	26
19	Applications of Ionic Liquids in Gas Processing **2012**, 133-138		1
18	On the viscosity of pyridinium based ionic liquids: an experimental and computational study. *Journal of Physical Chemistry B*, **2011**, 115, 12499-513	3.4	58
17	Theoretical Study of the Effect of Alkyl and Alkoxy Lateral Chains on the Structural and Electronic Properties of Conjugated Polymers Consisting of Phenylethynyl-1,3,4-thiadiazole. *Journal of Physical Chemistry C*, **2011**, 115, 2865-2873	3.8	42
16	Influence of the alkyl and alkoxy side chains on the electronic structure and charge-transport properties of polythiophene derivatives. *Physical Chemistry Chemical Physics*, **2011**, 13, 10091-9	3.6	10
15	Does the number of nitrogen atoms have an influence on the conducting properties of diphenylazines? A DFT insight. *Chemical Physics*, **2011**, 379, 51-56	2.3	6

14	Study on hydroxylammonium-based ionic liquids. I. Characterization. *Journal of Physical Chemistry B*, **2011**, 115, 12473-86	3.4	42
13	Optoelectronic and Charge Transport Properties of Oligomers Based on Phenylethynylene Units Linked to Thieno-acenes: A DFT Study. *Journal of Physical Chemistry C*, **2011**, 115, 6922-6932	3.8	29
12	Study on hydroxylammonium-based ionic liquids. II. Computational analysis of CO2 absorption. *Journal of Physical Chemistry B*, **2011**, 115, 12487-98	3.4	34
11	CO2 adsorption studies on hydroxy metal carbonates M(CO3)x(OH)y (M = Zn, Zn-Mg, Mg, Mg-Cu, Cu, Ni, and Pb) at high pressures up to 175 bar. *Langmuir*, **2011**, 27, 10642-7	4	38
10	The Role of Linear Alkyl and Alkoxy Side Chains in the Modulation of the Structure and Electrical Properties of Bithiophene:a Theoretical Study. *Australian Journal of Chemistry*, **2010**, 63, 1297	1.2	6
9	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. *Journal of Chemical Physics*, **2010**, 132, 064901	3.9	26
8	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, 5795-809	3.4	28
7	Review on the Use of Ionic Liquids (ILs) as Alternative Fluids for CO2Capture and Natural Gas Sweetening. *Energy & Fuels*, **2010**, 24, 5817-5828	4.1	396
6	Theoretical Study of Bis(phenylethynyl)thienoacenes as Precursors of Molecular Wires for Molecular Electronics. *Journal of Physical Chemistry C*, **2010**, 114, 12325-12334	3.8	18
5	Thermophysical Properties of Pure Ionic Liquids: Review of Present Situation. *Industrial & Engineering Chemistry Research*, **2010**, 49, 9580-9595	3.9	359
4	Computational Study of Hexamethylguanidinium Lactate Ionic Liquid: A Candidate for Natural Gas Sweetening. *Energy & Fuels*, **2010**, 24, 4989-5001	4.1	41
3	Force Transmission Error Analysis for a High-Pressure Single-Sinker Magnetic Suspension Densimeter. *International Journal of Thermophysics*, **2010**, 31, 698-709	2.1	20
2	Molecular structure, conformational preferences and vibrational analysis of 2-hydroxystyrene: A computational and spectroscopic research. *Chemical Physics*, **2010**, 374, 62-76	2.3	3
1	Theoretical study of the effect of ethynyl group on the structure and electrical properties of phenyl-thiadiazole systems as precursors of electron-conducting materials. *Journal of Chemical Physics*, **2009**, 130, 234907	3.9	28