Jos R B Gomes

List of Publications by Citations

230 papers	5,688 citations	40 h-index	55 g-index
246 ext. papers	6,355 ext. citations	5.1 avg, IF	6.11 L-index

#	Paper	IF	Citations
230	Understanding the reactivity of metallic nanoparticles: beyond the extended surface model for catalysis. *Chemical Society Reviews*, **2014**, 43, 4922-39	58.5	132
229	Accounting for van der Waals interactions between adsorbates and surfaces in density functional theory based calculations: selected examples. *RSC Advances*, **2013**, 3, 13085	3.7	120
228	Influence of step sites in the molecular mechanism of the water gas shift reaction catalyzed by copper. *Journal of Catalysis*, **2009**, 268, 131-141	7.3	88
227	"Recycling" classical drugs for malaria. *Chemical Reviews*, **2014**, 114, 11164-220	68.1	84
226	Density functional theory study of the water dissociation on platinum surfaces: general trends. *Journal of Physical Chemistry A*, **2014**, 118, 5832-40	2.8	82
225	Effect of the exchange-correlation potential and of surface relaxation on the description of the H(2)O dissociation on Cu(111). *Journal of Chemical Physics*, **2009**, 130, 224702	3.9	79
224	Good performance of the M06 family of hybrid meta generalized gradient approximation density functionals on a difficult case: CO adsorption on MgO(001). *Journal of Chemical Physics*, **2008**, 129, 124710	3.9	76
223	Structure of Chemisorbed CO(2) Species in Amine-Functionalized Mesoporous Silicas Studied by Solid-State NMR and Computer Modeling. *Journal of the American Chemical Society*, **2017**, 139, 389-408	16.4	75
222	Descriptors controlling the catalytic activity of metallic surfaces toward water splitting. *Journal of Catalysis*, **2010**, 276, 92-100	7.3	74
221	Theoretical study of bulk and surface oxygen and aluminum vacancies in Al2O3. *Physical Review B*, **2004**, 69,	3.3	74
220	A DFT study of the methanol oxidation catalyzed by a copper surface. *Surface Science*, **2001**, 471, 59-70	1.8	70
219	Salting-in with a salting-out agent: explaining the cation specific effects on the aqueous solubility of amino acids. *Journal of Physical Chemistry B*, **2013**, 117, 6116-28	3.4	65
218	Modeling adsorption in metal-organic frameworks with open metal sites: propane/propylene separations. *Langmuir*, **2012**, 28, 8537-49	4	64
217	Falcipains, Plasmodium falciparum cysteine proteases as key drug targets against malaria. *Current Medicinal Chemistry*, **2011**, 18, 1555-72	4.3	63
216	Computational approaches to study adsorption in MOFs with unsaturated metal sites. *Molecular Simulation*, **2014**, 40, 537-556	2	62
215	DFT Study of the CO Oxidation on the Au(321) Surface. *Journal of Physical Chemistry C*, **2008**, 112, 17291-17302	3.7	61
214	On the theoretical understanding of the unexpected O2 activation by nanoporous gold. *Chemical Communications*, **2011**, 47, 8403-5	5.8	60

213	Molecular dynamics simulation of diffusion coefficients and structural properties of ketones in supercritical CO 2 at infinite dilution. *Journal of Supercritical Fluids*, **2016**, 107, 630-638	4.2	59
212	Understanding Gas adsorption selectivity in IRMOF-8 using molecular simulation. *ACS Applied Materials & Interfaces*, **2015**, 7, 624-37	9.5	59
211	Adsorption of Atomic and Molecular Oxygen on the Au(321) Surface: DFT Study. *Journal of Physical Chemistry C*, **2007**, 111, 17311-17321	3.8	59
210	Molecular dynamics simulation studies of the interactions between ionic liquids and amino acids in aqueous solution. *Journal of Physical Chemistry B*, **2012**, 116, 1831-42	3.4	55
209	Standard molar enthalpies of formation, vapour pressures, and enthalpies of sublimation of 2-chloro-4-nitroaniline and 2-chloro-5-nitroaniline. *Journal of Chemical Thermodynamics*, **2003**, 35, 1343-1359	2.9	55
208	Amine functionalized porous silica for CO2/CH4 separation by adsorption: Which amine and why. *Chemical Engineering Journal*, **2018**, 336, 612-621	14.7	54
207	The structural relaxation of the □Al2O3(0001) □an investigation of potential errors. *Chemical Physics Letters*, **2001**, 341, 412-418	2.5	53
206	Control of crystallite and particle size in the synthesis of layered double hydroxides: Macromolecular insights and a complementary modeling tool. *Journal of Colloid and Interface Science*, **2016**, 468, 86-94	9.3	51
205	Solvent and Structural Effects in the N□H Bond Homolytic Dissociation Energy. *Journal of Physical Chemistry A*, **2004**, 108, 2119-2130	2.8	51
204	Density functional study of CO and NO adsorption on Ni-doped MgO(100). *Journal of Chemical Physics*, **2010**, 132, 104701	3.9	50
203	Adsorption of the formate species on copper surfaces: a DFT study. *Surface Science*, **1999**, 432, 279-290	1.8	50
202	Density functional theory model study of size and structure effects on water dissociation by platinum nanoparticles. *Journal of Chemical Physics*, **2012**, 137, 034701	3.9	49
201	MXenes as promising catalysts for water dissociation. *Applied Catalysis B: Environmental*, **2020**, 260, 118191	19.8	49
200	Accurate Model for Predicting Adsorption of Olefins and Paraffins on MOFs with Open Metal Sites. *Industrial & Engineering Chemistry Research*, **2014**, 53, 15475-15487	3.9	48
199	Enhancement of Ethane Selectivity in Ethane-Ethylene Mixtures by Perfluoro Groups in Zr-Based Metal-Organic Frameworks. *ACS Applied Materials & Interfaces*, **2019**, 11, 27410-27421	9.5	47
198	N-cinnamoylated chloroquine analogues as dual-stage antimalarial leads. *Journal of Medicinal Chemistry*, **2013**, 56, 556-67	8.3	46
197	On the geometric structure of the (0 0 0 1) hematite surface. *Surface Science*, **2004**, 558, 4-14	1.8	46
196	Corrosion inhibition of copper in aqueous chloride solution by 1H-1,2,3-triazole and 1,2,4-triazole and their combinations: electrochemical, Raman and theoretical studies. *Physical Chemistry Chemical Physics*, **2017**, 19, 6113-6129	3.6	44

195	DFT study of the adsorption of D-(L-)cysteine on flat and chiral stepped gold surfaces. *Langmuir*, **2013**, 29, 8856-64	4	44
194	Novel cinnamic acid/4-aminoquinoline conjugates bearing non-proteinogenic amino acids: towards the development of potential dual action antimalarials. *European Journal of Medicinal Chemistry*, **2012**, 54, 887-99	6.8	44
193	Surface model and exchange-correlation functional effects on the description of Pd/Al2O3(0001). *Journal of Chemical Physics*, **2002**, 116, 1684-1691	3.9	44
192	Vapor-Liquid Equilibria of Imidazolium Ionic Liquids with Cyano Containing Anions with Water and Ethanol. *Journal of Physical Chemistry B*, **2015**, 119, 10287-303	3.4	41
191	Combined experimental and computational study of the thermochemistry of the fluoroaniline isomers. *Journal of Physical Chemistry B*, **2007**, 111, 2052-61	3.4	40
190	Thermochemistry of nitronaphthalenes and nitroanthracenes. *Journal of Chemical Thermodynamics*, **2006**, 38, 748-755	2.9	40
189	Experimental and computational investigation of the energetics of the three isomers of monochloroaniline. *Journal of Physical Chemistry B*, **2005**, 109, 13356-62	3.4	40
188	Gas-Phase Thermodynamic Properties of Dichlorophenols Determined from Density Functional Theory Calculations. *Journal of Physical Chemistry A*, **2003**, 107, 869-874	2.8	40
187	Generalized BrnstedEvansPolanyi relationships and descriptors for OH bond cleavage of organic molecules on transition metal surfaces. *Journal of Catalysis*, **2014**, 313, 24-33	7.3	39
186	Combining multinuclear high-resolution solid-state MAS NMR and computational methods for resonance assignment of glutathione tripeptide. *Journal of Physical Chemistry A*, **2012**, 116, 6711-9	2.8	39
185	Bifunctional mixed-lanthanide cyano-bridged coordination polymers Ln(0.5)LnP(0.5)(H2O)5[W(CN)8] (Ln/LnP= Eu3+/Tb3+, Eu3+/Gd3+, Tb3+/Sm3+). *Inorganic Chemistry*, **2012**, 51, 9005-16	5.1	39
184	Viral surface glycoproteins, gp120 and gp41, as potential drug targets against HIV-1: brief overview one quarter of a century past the approval of zidovudine, the first anti-retroviral drug. *European Journal of Medicinal Chemistry*, **2011**, 46, 979-92	6.8	39
183	First-principles study of the adsorption of formaldehyde on the clean and atomic oxygen covered Cu(1 1 1) surface. *Journal of Molecular Catalysis A*, **2001**, 170, 187-193		39
182	Slow release of NO by microporous titanosilicate ETS-4. *Journal of the American Chemical Society*, **2011**, 133, 6396-402	16.4	38
181	The Role of Preadsorbed Atomic Hydrogen in the NO Dissociation on a Zigzag Stepped Gold Surface: A DFT Study. *Journal of Physical Chemistry C*, **2009**, 113, 8864-8877	3.8	38
180	Molecular simulation of silica/surfactant self-assembly in the synthesis of periodic mesoporous silicas. *Journal of the American Chemical Society*, **2007**, 129, 15414-5	16.4	38
179	Mechanistic Study of Carbon Monoxide Methanation over Pure and Rhodium- or Ruthenium-Doped Nickel Catalysts. *Journal of Physical Chemistry C*, **2015**, 119, 16537-16551	3.8	37
178	Interaction of CO2 and CH4 with Functionalized Periodic Mesoporous PhyleneSilica: Periodic DFT Calculations and Gas Adsorption Measurements. *Journal of Physical Chemistry C*, **2016**, 120, 3863-3875	3.8	36

177	Adsorption of Small Palladium Clusters on the Relaxed □Al2O3(0001) Surface. *Journal of Physical Chemistry B*, **2003**, 107, 6411-6424	3.4	36
176	Molecular dynamics simulation of the early stages of the synthesis of periodic mesoporous silica. *Journal of Physical Chemistry B*, **2009**, 113, 708-18	3.4	35
175	Experimental and computational study on the molecular energetics of indoline and indole. *Journal of Physical Chemistry A*, **2008**, 112, 12263-9	2.8	35
174	Novel insights into biomass delignification with acidic deep eutectic solvents: a mechanistic study of □O-4 ether bond cleavage and the role of the halide counterion in the catalytic performance. *Green Chemistry*, **2020**, 22, 2474-2487	10	34
173	Thermochemistry of some alkylsubstituted anthracenes. *Journal of Chemical Thermodynamics*, **2006**, 38, 367-375	2.9	34
172	Experimental and Computational Study on the Thermochemistry of Bromoanilines. *Bulletin of the Chemical Society of Japan*, **2006**, 79, 1852-1859	5.1	34
171	Water adsorption on a copper formate paddlewheel model of CuBTC: A comparative MP2 and DFT study. *Chemical Physics Letters*, **2013**, 587, 7-13	2.5	33
170	Modeling self-assembly of silica/surfactant mesostructures in the templated synthesis of nanoporous solids. *Langmuir*, **2013**, 29, 2387-96	4	33
169	Energetic studies and phase diagram of thioxanthene. *Journal of Physical Chemistry A*, **2009**, 113, 12988-94	2.8	33
168	Revisiting dibenzothiophene thermochemical data: Experimental and computational studies. *Journal of Chemical Thermodynamics*, **2009**, 41, 1199-1205	2.9	32
167	Gas-phase molecular structure and energetics of anionic silicates. *Geochimica Et Cosmochimica Acta*, **2008**, 72, 4421-4439	5.5	32
166	Combined experimental and computational study of the thermochemistry of methylpiperidines. *Journal of Organic Chemistry*, **2006**, 71, 3677-85	4.2	32
165	Thermochemistry of Small Organosulfur Compounds from ab Initio Calculations. *Journal of Physical Chemistry A*, **2004**, 108, 11684-11690	2.8	32
164	Facile Heterogeneously Catalyzed Nitrogen Fixation by MXenes. *ACS Catalysis*, **2020**, 10, 5049-5056	13.1	31
163	Toward an understanding of the aqueous solubility of amino acids in the presence of salts: a molecular dynamics simulation study. *Journal of Physical Chemistry B*, **2010**, 114, 16450-9	3.4	31
162	Topological analysis of the metal-support interaction: the case of Pd atoms on oxide surfaces. *Chemical Physics Letters*, **2004**, 388, 132-138	2.5	31
161	Comparative study of geometry and bonding character for methoxy radical adsorption on noble metals. *Computational and Theoretical Chemistry*, **2000**, 503, 189-200		31
160	Simple, mono and bifunctional periodic mesoporous organosilicas for removal of priority hazardous substances from water: The case of mercury(II). *Chemical Engineering Journal*, **2017**, 322, 263-274	14.7	30

159	Non-ionic hydrophobic eutectics versatile solvents for tailored metal separation and valorisation. *Green Chemistry*, **2020**, 22, 2810-2820	10	30
158	Unraveling the mechanism of the NO reduction by CO on gold based catalysts. *Journal of Catalysis*, **2012**, 289, 11-20	7.3	29
157	Ionic and radical adsorption on the Au(hkl) surfaces: A DFT study. *Surface Science*, **2012**, 606, 69-77	1.8	29
156	Cinnamic acid/chloroquinoline conjugates as potent agents against chloroquine-resistant Plasmodium falciparum. *ChemMedChem*, **2012**, 7, 1537-40	3.7	29
155	Density Functional Theory Study of Co, Rh, and Ir Atoms Deposited on the Al2O3(0001) Surface. *Journal of Physical Chemistry B*, **2004**, 108, 15671-15678	3.4	29
154	Gas-phase acidity of sulfonamides: implications for reactivity and prodrug design. *Tetrahedron*, **2005**, 61, 2705-2712	2.4	29
153	2- and 3-acetylpyrroles: a combined calorimetric and computational study. *Journal of Physical Chemistry A*, **2009**, 113, 3630-8	2.8	27
152	DFT study on the reaction of NO oxidation on a stepped gold surface. *Applied Catalysis A: General*, **2010**, 379, 111-120	5.1	27
151	Methoxy radical reaction to formaldehyde on clean and hydroxy radical-covered copper (111) surfaces: a density functional theory study. *Surface Science*, **1999**, 443, 165-176	1.8	27
150	Prediction of Ionic Liquids Properties through Molecular Dynamics Simulations. *Current Physical Chemistry*, **2014**, 4, 151-172	0.5	27
149	Improving the functionality and performance of AA2024 corrosion sensing coatings with nanocontainers. *Chemical Engineering Journal*, **2018**, 341, 526-538	14.7	26
148	Water Dissociation on Bimetallic Surfaces: General Trends. *Journal of Physical Chemistry C*, **2012**, 116, 10120-10128	3.8	26
147	The thermodynamics of the isomerization of cyanophenol and cyanothiophenol compounds. *Structural Chemistry*, **2007**, 18, 15-23	1.8	26
146	Reactivity of imidazolidin-4-one derivatives of primaquine: implications for prodrug design. *Tetrahedron*, **2006**, 62, 9883-9891	2.4	26
145	Density functional theory study on the thermodynamic properties of aminophenols. *International Journal of Quantum Chemistry*, **2005**, 101, 860-868	2.1	26
144	Adsorption of the formyl species on transition metal surfaces. *Journal of Electroanalytical Chemistry* , **2000**, 483, 180-187	4.1	26
143	Computational and experimental study of the behavior of cyano-based ionic liquids in aqueous solution. *Journal of Physical Chemistry B*, **2015**, 119, 1567-78	3.4	25
142	Energetic studies of two oxygen heterocyclic compounds Xanthone and tetrahydro-pyrone. *Journal of Thermal Analysis and Calorimetry*, **2009**, 97, 827-833	4.1	25

141	Experimental and computational study on the thermochemistry of the isomers of iodoaniline and diiodoaniline. *Chemical Physics Letters*, **2006**, 422, 565-570	2.5	25
140	Thermodynamic properties of quinoxaline-1,4-dioxide derivatives: a combined experimental and computational study. *Journal of Organic Chemistry*, **2004**, 69, 2785-92	4.2	25
139	A Transferable Model for Adsorption in MOFs with Unsaturated Metal Sites. *Journal of Physical Chemistry C*, **2017**, 121, 441-458	3.8	24
138	How Density Functional Theory Surface Energies May Explain the Morphology of Particles, Nanosheets, and Conversion Films Based on Layered Double Hydroxides. *Journal of Physical Chemistry C*, **2017**, 121, 2211-2220	3.8	24
137	New Model for Predicting Adsorption of Polar Molecules in Metal-Organic Frameworks with Unsaturated Metal Sites. *Journal of Physical Chemistry Letters*, **2018**, 9, 3544-3553	6.4	24
136	Cluster and periodic DFT calculations of adsorption of hydroxyl on the Au(h k l) surfaces. *Computational and Theoretical Chemistry*, **2010**, 946, 43-50		24
135	DFT study on the reaction of O2 dissociation catalyzed by gold surfaces doped with transition metal atoms. *Applied Catalysis A: General*, **2013**, 458, 90-102	5.1	23
134	Thermochemistry of bithiophenes and thienyl radicals. A calorimetric and computational study. *Journal of Physical Chemistry A*, **2009**, 113, 11042-50	2.8	23
133	Characterization of systems of thiophene and benzene with ionic liquids. *Journal of Molecular Liquids*, **2014**, 192, 26-31	6	22
132	Multiscale Model for the Templated Synthesis of Mesoporous Silica: The Essential Role of Silica Oligomers. *Chemistry of Materials*, **2016**, 28, 2715-2727	9.6	22
131	Unanticipated stereoselectivity in the reaction of primaquine alpha-aminoamides with substituted benzaldehydes: a computational and experimental study. *Journal of Organic Chemistry*, **2007**, 72, 4189-97	4.2	21
130	DFT study of the Au(321) surface reconstruction by consecutive deposition of oxygen atoms. *Surface Science*, **2008**, 602, 424-435	1.8	21
129	Thermochemistry of 2-amino-3-quinoxalinecarbonitrile-1,4-dioxide. Evaluation of the mean dissociation enthalpy of the (N-O) bond. *Organic and Biomolecular Chemistry*, **2004**, 2, 2507-12	3.9	21
128	Gas-phase thermochemistry of chloropyridines. *Chemical Physics Letters*, **2005**, 406, 154-160	2.5	21
127	Unravelling the Structure of Chemisorbed CO Species in Mesoporous Aminosilicas: A Critical Survey. *Environmental Science & Technology*, **2019**, 53, 2758-2767	10.3	20
126	"Washing-out" ionic liquids from polyethylene glycol to form aqueous biphasic systems. *Physical Chemistry Chemical Physics*, **2014**, 16, 2271-4	3.6	20
125	Experimental and Computational Studies on the Structural and Thermodynamic Properties of Two Sulfur Heterocyclic Keto Compounds. *Journal of Chemical & Engineering Data*, **2010**, 55, 5009-5017	2.8	20
124	Combined experimental and computational study of the energetics of methylindoles. *Journal of Chemical Thermodynamics*, **2009**, 41, 1193-1198	2.9	20

123	Energetic effects of ether and ketone functional groups in 9,10-dihydroanthracene compound. *Journal of Chemical Thermodynamics*, **2010**, 42, 1248-1254	2.9	20
122	Computational study on the bond dissociation enthalpies in the enolic and ketonic forms of beta-diketones: their influence on metal-ligand bond enthalpies. *Journal of Physical Chemistry A*, **2006**, 110, 13948-55	2.8	20
121	On the Need for Spin Polarization in Heterogeneously Catalyzed Reactions on Nonmagnetic Metallic Surfaces. *Journal of Chemical Theory and Computation*, **2012**, 8, 1737-43	6.4	19
120	Predicting hydration Gibbs energies of alkyl-aromatics using molecular simulation: a comparison of current force fields and the development of a new parameter set for accurate solvation data. *Physical Chemistry Chemical Physics*, **2011**, 13, 17384-94	3.6	19
119	Mechanism of ionic-liquid-based acidic aqueous biphasic system formation. *Physical Chemistry Chemical Physics*, **2018**, 20, 9838-9846	3.6	18
118	A molecular dynamics framework to explore the structure and dynamics of layered double hydroxides. *Applied Clay Science*, **2018**, 163, 164-177	5.2	18
117	Interaction of chitosan and chitin with Ni, Cu and Zn ions: A computational study. *Journal of Chemical Thermodynamics*, **2014**, 73, 121-129	2.9	18
116	A computational study on the energetics and reactivity of some xanthene and thioxanthene derivatives. *Structural Chemistry*, **2013**, 24, 661-670	1.8	18
115	Fischer-Tropsch Synthesis on Multicomponent Catalysts: What Can We Learn from Computer Simulations?. *Catalysts*, **2015**, 5, 3-17	4	18
114	Molecular energetics of 4-methyldibenzothiophene: An experimental study. *Journal of Chemical Thermodynamics*, **2010**, 42, 251-255	2.9	18
113	Experimental and computational studies on the molecular energetics of chlorobenzophenones. *Journal of Physical Chemistry B*, **2007**, 111, 13033-40	3.4	18
112	Molecular energetics of cytosine revisited: a joint computational and experimental study. *Journal of Physical Chemistry A*, **2007**, 111, 7237-42	2.8	18
111	Combined experimental and computational thermochemistry of isomers of chloronitroanilines. *Journal of Chemical Thermodynamics*, **2008**, 40, 155-165	2.9	18
110	The effect of atomic point charges on adsorption isotherms of CO2 and water in metal organic frameworks. *Adsorption*, **2020**, 26, 663-685	2.6	18
109	Molecular Simulations of the Synthesis of Periodic Mesoporous Silica Phases at High Surfactant Concentrations. *Journal of Physical Chemistry C*, **2017**, 121, 4564-4575	3.8	17
108	Insights into CO2 and CH4 Adsorption by Pristine and Aromatic Amine-Modified Periodic Mesoporous Phenylene-Silicas. *Journal of Physical Chemistry C*, **2016**, 120, 14236-14245	3.8	17
107	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (ROH, COOH, CONH2). *Journal of Chemical Thermodynamics*, **2012**, 54, 108-117	2.9	17
106	1H-1H double-quantum CRAMPS NMR at very-fast MAS (nuR=35 kHz): a resolution enhancement method to probe 1H-1H proximities in solids. *Journal of Magnetic Resonance*, **2009**, 196, 88-91	3	17

105	Comparative computational and experimental study on the thermochemistry of the chloropyrimidines. *Journal of Physical Chemistry B*, **2007**, 111, 792-9	3.4	17
104	Cluster model study of methoxy radical adsorption on the Cu (111) surface. *Computational and Theoretical Chemistry*, **1999**, 463, 163-168		17
103	Development of Plasmodium falciparum protease inhibitors in the past decade (2002-2012). *Current Medicinal Chemistry*, **2013**, 20, 3049-68	4.3	17
102	First-Principles Calculations on the Adsorption Behavior of Amino Acids on a Titanium Carbide MXene.. *ACS Applied Bio Materials*, **2020**, 3, 5913-5921	4.1	17
101	Evidence for the interactions occurring between ionic liquids and tetraethylene glycol in binary mixtures and aqueous biphasic systems. *Journal of Physical Chemistry B*, **2014**, 118, 4615-29	3.4	16
100	Universal model for accurate calculation of tracer diffusion coefficients in gas, liquid and supercritical systems. *Journal of Chromatography A*, **2013**, 1290, 1-26	4.5	16
99	Experimental and computational investigation of the thermochemistry of the six isomers of dichloroaniline. *Journal of Physical Chemistry A*, **2006**, 110, 9301-6	2.8	16
98	Adsorption of Ar atoms on the relaxed defect-free TiO2(110) surface. *Physical Review B*, **2005**, 71,	3.3	16
97	A theoretical study of dioxymethylene, proposed as intermediate in the oxidation of formaldehyde to formate over copper. *Surface Science*, **2000**, 446, 283-293	1.8	16
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94	Structural, energetic and reactivity properties of phenoxazine and phenothiazine. *Journal of Chemical Thermodynamics*, **2014**, 73, 110-120	2.9	15
93	Effect of van der Waals interactions in the DFT description of self-assembled monolayers of thiols on gold. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	15
92	The origin of the LCST on the liquid-liquid equilibrium of thiophene with ionic liquids. *Journal of Physical Chemistry B*, **2012**, 116, 5985-92	3.4	15
91	Thermochemical studies on 3-methyl-quinoxaline-2-carboxamide-1,4-dioxide derivatives: enthalpies of formation and of N-O bond dissociation. *Journal of Physical Chemistry B*, **2007**, 111, 2075-80	3.4	15
90	Energetics of the N-O bonds in 2-hydroxyphenazine-di-N-oxide. *Journal of Physical Chemistry B*, **2005**, 109, 16188-95	3.4	15
89	Effect of the Exchange-Correlation Potential on the Transferability of Brønsted-Evans-Polanyi Relationships in Heterogeneous Catalysis. *Journal of Chemical Theory and Computation*, **2016**, 12, 2121-6	6.4	15
88	Mechanisms of phase separation in temperature-responsive acidic aqueous biphasic systems. *Physical Chemistry Chemical Physics*, **2019**, 21, 7462-7473	3.6	14

87	Elucidating StructureProperty Relationships in Aluminum Alloy Corrosion Inhibitors by Machine Learning. *Journal of Physical Chemistry C*, **2020**, 124, 5624-5635	3.8	14
86	Energetics and Reactivity of Morpholine and Thiomorpholine: A Joint Experimental and Computational Study. *Journal of Chemical & Engineering Data*, **2014**, 59, 312-322	2.8	14
85	Dibenzofuran and methyldibenzofuran derivatives: assessment of thermochemical data. *Structural Chemistry*, **2013**, 24, 1923-1933	1.8	14
84	DFT study on the NO oxidation on a flat gold surface model. *Chemical Physics Letters*, **2011**, 503, 129-133	2.5	14
83	Theoretical study on the stability of formylphenol and formylaniline compounds and corresponding radicals: O-H or N-H vs C-H bond dissociation. *Journal of Physical Chemistry A*, **2009**, 113, 1628-34	2.8	14
82	Quinoxaline-1,4-dioxide: Substituent effects on the N O bond dissociation enthalpy. *Chemical Physics Letters*, **2006**, 429, 18-22	2.5	14
81	Kinetics and mechanism of hydrolysis of N-acyloxymethyl derivatives of azetidin-2-one. *Journal of Organic Chemistry*, **2004**, 69, 3359-67	4.2	14
80	MXenes atomic layer stacking phase transitions and their chemical activity consequences. *Physical Review Materials*, **2020**, 4,	3.2	14
79	A computational UV Vis spectroscopic study of the chemical speciation of 2-mercaptobenzothiazole corrosion inhibitor in aqueous solution. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	14
78	Pyrolyzed chitosan-based materials for CO2/CH4 separation. *Chemical Engineering Journal*, **2019**, 362, 364-374	14.7	14
77	Modelling the self-assembly of silica-based mesoporous materials. *Molecular Simulation*, **2018**, 44, 435-452		13
76	Adsorption of Xe atoms on the TiO2(110) surface: A density functional study. *Surface Science*, **2010**, 604, 428-434	1.8	13
75	Multifunctionality in an Ion-Exchanged Porous Metal-Organic Framework. *Journal of the American Chemical Society*, **2021**, 143, 1365-1376	16.4	13
74	Selectivity for CO2 over CH4 on a functionalized periodic mesoporous phenylene-silica explained by transition state theory. *Chemical Physics Letters*, **2017**, 671, 161-164	2.5	12
73	Carbonization of periodic mesoporous phenylene- and biphenylene-silicas for CO2/CH4 separation. *Carbon*, **2017**, 119, 267-277	10.4	12
72	Periodic mesoporous organosilica with low thiol density a safer material to trap Hg(II) from water. *Journal of Environmental Chemical Engineering*, **2017**, 5, 5043-5053	6.8	12
71	A computational study on the thermochemistry of methylbenzo- and methyldibenzothiophenes. *Computational and Theoretical Chemistry*, **2010**, 946, 20-25		12
70	Experimental and computational study of the thermochemistry of the fluoromethylaniline isomers. *Journal of Physical Chemistry B*, **2007**, 111, 6444-51	3.4	12

69	The adsorption of methyl nitrite on the Au(111) surface. *Catalysis Letters*, **2001**, 71, 31-35	2.8	12
68	Microwave-assisted N,N-dialkylation of amine-functionalized periodic mesoporous phenylene-silica: An easy and fast way to design materials. *Microporous and Mesoporous Materials*, **2017**, 249, 10-15	5.3	11
67	Optimization of the time and temperature of the microwave-assisted amination of phenylene-PMO. *RSC Advances*, **2015**, 5, 9208-9216	3.7	11
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