Jos R B Gomes

List of Publications by Year in Descending Order

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	Moisture effect on the separation of CO2/CH4 mixtures with amine-functionalised porous silicas. *Chemical Engineering Journal*, **2022**, 136271	14.7	1
229	The dipole moment of alcohols in the liquid phase and in solution. *Journal of Molecular Liquids*, **2022**, 356, 119033	6	2
228	CO2 and CH4 adsorption on periodic mesoporous organosilica: A DFT study. *Materials Today Communications*, **2021**, 26, 102088	2.5	2
227	The Ti2CO2 MXene as a nucleobase 2D sensor: A first-principles study. *Applied Surface Science*, **2021**, 544, 148946	6.7	5
226	Exploring periodic mesoporous organosilicas for ethane–ethylene adsorption–separation. *Microporous and Mesoporous Materials*, **2021**, 317, 110975	5.3	2
225	Concepts, models, and methods in computational heterogeneous catalysis illustrated through CO2 conversion. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1530	7.9	11
224	Self-consistent electrostatic embedding for liquid phase polarization. *Journal of Molecular Liquids*, **2021**, 322, 114550	6	3
223	Revisiting Tracer Liu-Silva-Macedo model for binary diffusion coefficient using the largest database of liquid and supercritical systems. *Journal of Supercritical Fluids*, **2021**, 168, 105073	4.2	1
222	Multifunctionality in an Ion-Exchanged Porous Metal-Organic Framework. *Journal of the American Chemical Society*, **2021**, 143, 1365-1376	16.4	13
221	Unravelling moisture-induced CO chemisorption mechanisms in amine-modified sorbents at the molecular scale. *Journal of Materials Chemistry A*, **2021**, 9, 5542-5555	13	11
220	Diffusion of quercetin in compressed liquid ethyl acetate and ethanol. *Journal of Molecular Liquids*, **2021**, 324, 114714	6	1
219	Catalytic reactions for H2 production on multimetallic surfaces: a review. *JPhys Energy*, **2021**, 3, 032016	4.9	2
218	Carbon Capture and Usage by MXenes. *ACS Catalysis*, **2021**, 11, 11248-11255	13.1	8
217	New Force-Field for Organosilicon Molecules in the Liquid Phase.. *ACS Physical Chemistry Au*, **2021**, 1, 54-69		0
216	Surface-Enhanced Raman Scattering due to a Synergistic Effect on ZnS and Graphene Oxide. *Journal of Physical Chemistry C*, **2020**, 124, 12742-12751	3.8	6
215	Non-ionic hydrophobic eutectics – versatile solvents for tailored metal separation and valorisation. *Green Chemistry*, **2020**, 22, 2810-2820	10	30
214	The cation effect on the solubility of glycylglycine and N-acetylglycine in aqueous solution: Experimental and molecular dynamics studies. *Journal of Molecular Liquids*, **2020**, 310, 113044	6	1

213	Novel insights into biomass delignification with acidic deep eutectic solvents: a mechanistic study of β-O-4 ether bond cleavage and the role of the halide counterion in the catalytic performance. *Green Chemistry*, **2020**, 22, 2474-2487	10	34
212	Elucidating Structure–Property Relationships in Aluminum Alloy Corrosion Inhibitors by Machine Learning. *Journal of Physical Chemistry C*, **2020**, 124, 5624-5635	3.8	14
211	Emerging trends in smart nanocontainers for corrosion applications **2020**, 385-398		5
210	Cinnamic Derivatives as Antitubercular Agents: Characterization by Quantitative Structure-Activity Relationship Studies. *Molecules*, **2020**, 25,	4.8	4
209	Facile Heterogeneously Catalyzed Nitrogen Fixation by MXenes. *ACS Catalysis*, **2020**, 10, 5049-5056	13.1	31
208	MXenes atomic layer stacking phase transitions and their chemical activity consequences. *Physical Review Materials*, **2020**, 4,	3.2	14
207	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
206	A computational study of the interaction of C2 hydrocarbons with CuBTC. *Computational Materials Science*, **2020**, 173, 109438	3.2	1
205	Unveiling the local structure of 2-mercaptobenzothiazole intercalated in (Zn2Al) layered double hydroxides. *Applied Clay Science*, **2020**, 198, 105842	5.2	2
204	Mesoscale model of the synthesis of periodic mesoporous benzene-silica. *Journal of Molecular Liquids*, **2020**, 316, 113861	6	2
203	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
202	MXenes as promising catalysts for water dissociation. *Applied Catalysis B: Environmental*, **2020**, 260, 118191	21.8	49
201	Measurement of astaxanthin and squalene diffusivities in compressed liquid ethyl acetate by Taylor-Aris dispersion method. *Separation and Purification Technology*, **2020**, 234, 116046	8.3	2
200	Mechanisms of phase separation in temperature-responsive acidic aqueous biphasic systems. *Physical Chemistry Chemical Physics*, **2019**, 21, 7462-7473	3.6	14
199	Unravelling the Structure of Chemisorbed CO Species in Mesoporous Aminosilicas: A Critical Survey. *Environmental Science & Technology*, **2019**, 53, 2758-2767	10.3	20
198	A DFT study on the interaction of small molecules with alkali metal ion-exchanged ETS-10. *Zeitschrift Fur Kristallographie - Crystalline Materials*, **2019**, 234, 483-493	1	1
197	Implicit solvent effects in the determination of Brønsted-Evans-Polanyi relationships for heterogeneously catalyzed reactions. *Physical Chemistry Chemical Physics*, **2019**, 21, 17687-17695	3.6	3
196	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

195	Pyrolyzed chitosan-based materials for CO2/CH4 separation. *Chemical Engineering Journal*, **2019**, 362, 364-374	14.7	14
194	Hydrogen bonding networks in gabapentin protic pharmaceutical salts: NMR and in silico studies. *Magnetic Resonance in Chemistry*, **2019**, 57, 243-255	2.1	1
193	Mechanism of ionic-liquid-based acidic aqueous biphasic system formation. *Physical Chemistry Chemical Physics*, **2018**, 20, 9838-9846	3.6	18
192	Improving the functionality and performance of AA2024 corrosion sensing coatings with nanocontainers. *Chemical Engineering Journal*, **2018**, 341, 526-538	14.7	26
191	Modelling the self-assembly of silica-based mesoporous materials. *Molecular Simulation*, **2018**, 44, 435-452		13
190	A molecular dynamics framework to explore the structure and dynamics of layered double hydroxides. *Applied Clay Science*, **2018**, 163, 164-177	5.2	18
189	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
188	Amine functionalized porous silica for CO2/CH4 separation by adsorption: Which amine and why. *Chemical Engineering Journal*, **2018**, 336, 612-621	14.7	54
187	Flue gas adsorption on periodic mesoporous phenylene-silica: a DFT approach. *Physical Chemistry Chemical Physics*, **2018**, 20, 16686-16694	3.6	9
186	Understanding Polymorphic Control of Pharmaceuticals Using Imidazolium-Based Ionic Liquid Mixtures as Crystallization Directing Agents. *Crystal Growth and Design*, **2017**, 17, 428-432	3.5	15
185	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
184	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
183	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
182	Carbonization of periodic mesoporous phenylene- and biphenylene-silicas for CO2/CH4 separation. *Carbon*, **2017**, 119, 267-277	10.4	12
181	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
180	Thermochemical studies on two alkyl-bulky substituted xanthene derivatives: 9,9-dimethylxanthene and 2,7-di-tert-butyl-9,9-dimethylxanthene. *Journal of Chemical Thermodynamics*, **2017**, 106, 168-177	2.9	5
179	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
178	A Transferable Model for Adsorption in MOFs with Unsaturated Metal Sites. *Journal of Physical Chemistry C*, **2017**, 121, 441-458	3.8	24

177	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
176	Adsorption of CO on the rutile TiO(110) surface: a dispersion-corrected density functional theory study. *Physical Chemistry Chemical Physics*, **2017**, 19, 2487-2494	3.6	8
175	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
174	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
173	Energetic and reactivity properties of 9,10-dihydroacridine and diphenylamine: A comparative overview. *Journal of Chemical Thermodynamics*, **2017**, 115, 276-284	2.9	3
172	Gas-Organic and Gas-Inorganic Interfacial Effects in Gas/Adsorbent Interactions: The Case of CO2 /CH4 Separation **2017**, 413-458		1
171	Water dissociation on multimetallic catalysts. *Applied Catalysis B: Environmental*, **2017**, 218, 199-207	21.8	11
170	Prediction of metallic nanotube reactivity for HO activation. *Physical Chemistry Chemical Physics*, **2017**, 19, 19188-19195	3.6	1
169	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
168	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
167	Why are some cyano-based ionic liquids better glucose solvents than water?. *Physical Chemistry Chemical Physics*, **2016**, 18, 18958-70	3.6	11
166	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
165	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
164	Methanol dissociation on bimetallic surfaces: validity of the general BrEvansPolanyi relationship for OH bond cleavage. *RSC Advances*, **2016**, 6, 18695-18702	3.7	10
163	Striking HIV-1 Entry by Targeting HIV-1 gp41. But, Where Should We Target?. *PLoS ONE*, **2016**, 11, e0146743	3.7	
162	A computational UVVis spectroscopic study of the chemical speciation of 2-mercaptobenzothiazole corrosion inhibitor in aqueous solution. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	14
161	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
160	Effect of the Exchange-Correlation Potential on the Transferability of Br-Evans-Polanyi Relationships in Heterogeneous Catalysis. *Journal of Chemical Theory and Computation*, **2016**, 12, 2121-6	6.4	15

159	Understanding the cation specific effects on the aqueous solubility of amino acids: from mono to polyvalent cations. *RSC Advances*, **2015**, 5, 15024-15034	3.7	7
158	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
157	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
156	A density functional theory study on the interaction of paraffins, olefins, and acetylenes with Na-ETS-10. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	4
155	Turning periodic mesoporous organosilicas selective to CO2/CH4 separation: deposition of aluminium oxide by atomic layer deposition. *Journal of Materials Chemistry A*, **2015**, 3, 22860-22867	13	15
154	Optimization of the time and temperature of the microwave-assisted amination of phenylene-PMO. *RSC Advances*, **2015**, 5, 9208-9216	3.7	11
153	Evaluation of the GROMOS 56ACARBO Force Field for the Calculation of Structural, Volumetric, and Dynamic Properties of Aqueous Glucose Systems. *Journal of Physical Chemistry B*, **2015**, 119, 15310-9	3.4	10
152	Understanding Gas adsorption selectivity in IRMOF-8 using molecular simulation. *ACS Applied Materials & Interfaces*, **2015**, 7, 624-37	9.5	59
151	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
150	Fischer-Tropsch Synthesis on Multicomponent Catalysts: What Can We Learn from Computer Simulations?. *Catalysts*, **2015**, 5, 3-17	4	18
149	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
148	Computational approaches to study adsorption in MOFs with unsaturated metal sites. *Molecular Simulation*, **2014**, 40, 537-556	2	62
147	Understanding the reactivity of metallic nanoparticles: beyond the extended surface model for catalysis. *Chemical Society Reviews*, **2014**, 43, 4922-39	58.5	132
146	Generalized Brønsted–Evans–Polanyi relationships and descriptors for O–H bond cleavage of organic molecules on transition metal surfaces. *Journal of Catalysis*, **2014**, 313, 24-33	7.3	39
145	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
144	"Recycling" classical drugs for malaria. *Chemical Reviews*, **2014**, 114, 11164-220	68.1	84
143	"Washing-out" ionic liquids from polyethylene glycol to form aqueous biphasic systems. *Physical Chemistry Chemical Physics*, **2014**, 16, 2271-4	3.6	20
142	Molecular simulation of the adsorption of methane in Engelhard titanosilicate frameworks. *Langmuir*, **2014**, 30, 7435-46	4	6

141	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
140	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
139	Interaction of atmospheric gases with ETS-10: A DFT study. *Microporous and Mesoporous Materials*, **2014**, 190, 38-45	5.3	8
138	Characterization of systems of thiophene and benzene with ionic liquids. *Journal of Molecular Liquids*, **2014**, 192, 26-31	6	22
137	Structural, energetic and reactivity properties of phenoxazine and phenothiazine. *Journal of Chemical Thermodynamics*, **2014**, 73, 110-120	2.9	15
136	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
135	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
134	Prediction of Ionic Liquids Properties through Molecular Dynamics Simulations. *Current Physical Chemistry*, **2014**, 4, 151-172	0.5	27
133	Structures and energetics of organosilanes in the gaseous phase: a computational study. *Highlights in Theoretical Chemistry*, **2014**, 167-176		
132	Structures and energetics of organosilanes in the gaseous phase: a computational study. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	6
131	DFT study of the adsorption of D-(L-)cysteine on flat and chiral stepped gold surfaces. *Langmuir*, **2013**, 29, 8856-64	4	44
130	Dibenzofuran and methyldibenzofuran derivatives: assessment of thermochemical data. *Structural Chemistry*, **2013**, 24, 1923-1933	1.8	14
129	A computational study on the energetics and reactivity of some xanthene and thioxanthene derivatives. *Structural Chemistry*, **2013**, 24, 661-670	1.8	18
128	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
127	Toward the discovery of inhibitors of babesipain-1, a Babesia bigemina cysteine protease: in vitro evaluation, homology modeling and molecular docking studies. *Journal of Computer-Aided Molecular Design*, **2013**, 27, 823-35	4.2	5
126	Modeling self-assembly of silica/surfactant mesostructures in the templated synthesis of nanoporous solids. *Langmuir*, **2013**, 29, 2387-96	4	33
125	N-cinnamoylated chloroquine analogues as dual-stage antimalarial leads. *Journal of Medicinal Chemistry*, **2013**, 56, 556-67	8.3	46
124	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

123	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
122	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
121	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
120	A DFT study of the NO dissociation on gold surfaces doped with transition metals. *Journal of Chemical Physics*, **2013**, 138, 074701	3.9	9
119	Role of the organic linker in the early stages of the templated synthesis of PMOs. *Physical Chemistry Chemical Physics*, **2013**, 15, 6166-9	3.6	6
118	Efeitos energ□tico-estruturais em compostos heteropolic□licos com oxig□io ou enxofre. *Quimica Nova*, **2013**, 36, 840-847	1.6	7
117	Development of Plasmodium falciparum protease inhibitors in the past decade (2002-2012). *Current Medicinal Chemistry*, **2013**, 20, 3049-68	4.3	17
116	Unraveling the mechanism of the NO reduction by CO on gold based catalysts. *Journal of Catalysis*, **2012**, 289, 11-20	7.3	29
115	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
114	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
113	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
112	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
111	Ionic and radical adsorption on the Au(hkl) surfaces: A DFT study. *Surface Science*, **2012**, 606, 69-77	1.8	29
110	Experimental and computational thermochemical studies of 9-R-xanthene derivatives (ROH, COOH, CONH2). *Journal of Chemical Thermodynamics*, **2012**, 54, 108-117	2.9	17
109	Modeling adsorption in metal-organic frameworks with open metal sites: propane/propylene separations. *Langmuir*, **2012**, 28, 8537-49	4	64
108	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
107	Water Dissociation on Bimetallic Surfaces: General Trends. *Journal of Physical Chemistry C*, **2012**, 116, 10120-10128	3.8	26
106	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

105	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
104	Synthesis and thermochemical study of quinoxaline-N-oxides: enthalpies of dissociation of the N□O bond. *Journal of Physical Organic Chemistry*, **2012**, 25, 420-426	2.1	5
103	Cinnamic acid/chloroquinoline conjugates as potent agents against chloroquine-resistant Plasmodium falciparum. *ChemMedChem*, **2012**, 7, 1537-40	3.7	29
102	Slow release of NO by microporous titanosilicate ETS-4. *Journal of the American Chemical Society*, **2011**, 133, 6396-402	16.4	38
101	On the theoretical understanding of the unexpected O2 activation by nanoporous gold. *Chemical Communications*, **2011**, 47, 8403-5	5.8	60
100	Catalytic Reactions on Model Gold Surfaces: Effect of Surface Steps and of Surface Doping. *Catalysts*, **2011**, 1, 40-51	4	4
99	Thermochemistry of TM(II) Complexes (TM=Ni, Cu and Zn) and Their Ligands from DFT Calculations. *Current Physical Chemistry*, **2011**, 1, 55-64	0.5	1
98	Molecular docking and 3D-quantitative structure activity relationship analyses of peptidyl vinyl sulfones: Plasmodium Falciparum cysteine proteases inhibitors. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 763-75	4.2	7
97	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
96	DFT study on the NO oxidation on a flat gold surface model. *Chemical Physics Letters*, **2011**, 503, 129-133	2.5	14
95	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
94	Falcipains, Plasmodium falciparum cysteine proteases as key drug targets against malaria. *Current Medicinal Chemistry*, **2011**, 18, 1555-72	4.3	63
93	Density functional study of CO and NO adsorption on Ni-doped MgO(100). *Journal of Chemical Physics*, **2010**, 132, 104701	3.9	50
92	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
91	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
90	Energetic effects of ether and ketone functional groups in 9,10-dihydroanthracene compound. *Journal of Chemical Thermodynamics*, **2010**, 42, 1248-1254	2.9	20
89	Descriptors controlling the catalytic activity of metallic surfaces toward water splitting. *Journal of Catalysis*, **2010**, 276, 92-100	7.3	74
88	Molecular energetics of 4-methyldibenzothiophene: An experimental study. *Journal of Chemical Thermodynamics*, **2010**, 42, 251-255	2.9	18

87	Water adsorption and dissociation on the Au(321) stepped surface. *Computational and Theoretical Chemistry*, **2010**, 946, 51-56		11
86	A computational study on the thermochemistry of methylbenzo- and methyldibenzothiophenes. *Computational and Theoretical Chemistry*, **2010**, 946, 20-25		12
85	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
84	Adsorption of Xe atoms on the TiO2(110) surface: A density functional study. *Surface Science*, **2010**, 604, 428-434	1.8	13
83	DFT study on the reaction of NO oxidation on a stepped gold surface. *Applied Catalysis A: General*, **2010**, 379, 111-120	5.1	27
82	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
81	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
80	Energetic studies of two oxygen heterocyclic compounds Xanthone and tetrahydro-4-pyrone. *Journal of Thermal Analysis and Calorimetry*, **2009**, 97, 827-833	4.1	25
79	The enthalpies of dissociation of the N?O bonds in two quinoxaline derivatives. *Journal of Physical Organic Chemistry*, **2009**, 22, 17-23	2.1	6
78	Combined experimental and computational study of the energetics of methylindoles. *Journal of Chemical Thermodynamics*, **2009**, 41, 1193-1198	2.9	20
77	Revisiting dibenzothiophene thermochemical data: Experimental and computational studies. *Journal of Chemical Thermodynamics*, **2009**, 41, 1199-1205	2.9	32
76	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
75	2- and 3-acetylpyrroles: a combined calorimetric and computational study. *Journal of Physical Chemistry A*, **2009**, 113, 3630-8	2.8	27
74	Energetic studies and phase diagram of thioxanthene. *Journal of Physical Chemistry A*, **2009**, 113, 12988-94	2.8	33
73	Thermochemistry of bithiophenes and thienyl radicals. A calorimetric and computational study. *Journal of Physical Chemistry A*, **2009**, 113, 11042-50	2.8	23
72	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
71	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
70	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

69	Experimental and computational study on the molecular energetics of indoline and indole. *Journal of Physical Chemistry A*, **2008**, 112, 12263-9	2.8	35
68	Gas-phase molecular structure and energetics of anionic silicates. *Geochimica Et Cosmochimica Acta*, **2008**, 72, 4421-4439	5.5	32
67	Azomethane Decomposition Catalyzed by Pt(111): An Example of Anti-Brønsted-Evans-Polanyi Behavior. *Journal of Physical Chemistry C*, **2008**, 112, 1072-1080	3.8	5
66	DFT Study of the CO Oxidation on the Au(321) Surface. *Journal of Physical Chemistry C*, **2008**, 112, 17291-17302	3.8	61
65	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
64	Standard molar enthalpies of formation of dimethylbenzophenones. *Journal of Physical Organic Chemistry*, **2008**, 21, 365-371	2.1	2
63	Combined experimental and computational thermochemistry of isomers of chloronitroanilines. *Journal of Chemical Thermodynamics*, **2008**, 40, 155-165	2.9	18
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