

Robin Chaudret

List of Publications by Year in descending order

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21
papers

3,540
citations

759233

12
h-index

752698

20
g-index

21
all docs

21
docs citations

21
times ranked

4450
citing authors

#	ARTICLE	IF	CITATIONS
1	A Complete NCI Perspective: From New Bonds to Reactivity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 491-527.	0.6	24
2	Influence of the Precursor Composition and Reaction Conditions on Raney-Nickel Catalytic System. Molecular Modeling and Simulation, 2016, , 125-135.	0.2	0
3	Molecular modeling and simulation of Raney Nickel: From alloy precursor to the final porous catalyst. Computational Materials Science, 2015, 99, 336-342.	3.0	9
4	Addressing the Issues of Non-isotropy and Non-additivity in the Development of Quantum Chemistry-Grounded Polarizable Molecular Mechanics. Challenges and Advances in Computational Chemistry and Physics, 2015, , 1-49.	0.6	1
5	Revisiting H ₂ O Nucleation around Au ⁺ and Hg ²⁺ : The Peculiar "Pseudo-Soft" Character of the Gold Cation. Journal of Chemical Theory and Computation, 2014, 10, 1900-1909.	5.3	7
6	S/G-1: An ab Initio Force-Field Blending Frozen Hermite Gaussian Densities and Distributed Multipoles. Proof of Concept and First Applications to Metal Cations. Journal of Physical Chemistry A, 2014, 118, 7598-7612.	2.5	22
7	Nonclassical CH ^{δ+} Supramolecular Interactions in Artemisinic Acid Favor a Single Conformation, Yielding High Diastereoselectivity in the Reduction with Diazene. Journal of Organic Chemistry, 2014, 79, 5939-5947.	3.2	13
8	Impact of functionalized linkers on the energy landscape of ZIFs. CrystEngComm, 2013, 15, 9603.	2.6	28
9	Noncovalent Interaction Analysis in Fluctuating Environments. Journal of Chemical Theory and Computation, 2013, 9, 2226-2234.	5.3	150
10	Toward a Deeper Understanding of Enzyme Reactions Using the Coupled ELF/NCI Analysis: Application to DNA Repair Enzymes. Journal of Chemical Theory and Computation, 2013, 9, 2156-2160.	5.3	48
11	Further refinements of next-generation force fields " Nonempirical localization of off-centered points in molecules. Canadian Journal of Chemistry, 2013, 91, 804-810.	1.1	10
12	Pseudobond parameters for QM/MM studies involving nucleosides, nucleotides, and their analogs. Journal of Chemical Physics, 2013, 138, 045102.	3.0	5
13	Catalytic Mechanism of 4-Oxalocrotonate Tautomerase: Significances of Protein-Protein Interactions on Proton Transfer Pathways. Journal of Physical Chemistry B, 2012, 116, 6889-6897.	2.6	7
14	Coupling Quantum Interpretative Techniques: Another Look at Chemical Mechanisms in Organic Reactions. Journal of Chemical Theory and Computation, 2012, 8, 3993-3997.	5.3	104
15	Toward a ligand specific of Pb ²⁺ with respect to the Zn ²⁺ and Ca ²⁺ cations: A track from quantum chemistry. Chemical Physics Letters, 2012, 532, 9-12.	2.6	2
16	Electron Pair Localization Function (EPLF) for Density Functional Theory and <i>ab Initio</i> Wave Function-Based Methods: A New Tool for Chemical Interpretation. Journal of Chemical Theory and Computation, 2011, 7, 618-624.	5.3	17
17	Correlation between electron localization and metal ion mutagenicity in DNA synthesis from QM/MM calculations. Physical Chemistry Chemical Physics, 2011, 13, 11239.	2.8	18
18	NCIPLLOT: A Program for Plotting Noncovalent Interaction Regions. Journal of Chemical Theory and Computation, 2011, 7, 625-632.	5.3	2,897

#	ARTICLE	IF	CITATIONS
19	Many-body exchange-repulsion in polarizable molecular mechanics. I. orbital-based approximations and applications to hydrated metal cation complexes. <i>Journal of Computational Chemistry</i> , 2011, 32, 2949-2957.	3.3	30
20	Unraveling Low-Barrier Hydrogen Bonds in Complex Systems with a Simple Quantum Topological Criterion. <i>Chemistry - A European Journal</i> , 2011, 17, 2833-2837.	3.3	11
21	Polarizable Molecular Dynamics Simulation of Zn(II) in Water Using the AMOEBA Force Field. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2059-2070.	5.3	137