

# Camelia Muñoz-Caro

## List of Publications by Year in descending order

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67  
papers

1,114  
citations

394421

19  
h-index

414414

32  
g-index

67  
all docs

67  
docs citations

67  
times ranked

980  
citing authors

#	ARTICLE	IF	CITATIONS
1	A fine-grained loop-level parallel approach to efficient fuzzy community detection in complex networks. <i>Concurrency Computation Practice and Experience</i> , 2020, 32, e5537.	2.2	0
2	A General Approach to Fuzzy Community Detection in Social Networks. , 2019, , .		2
3	Refinement of a generalized Fermat's last theorem conjecture in natural vector spaces. <i>Journal of Mathematical Chemistry</i> , 2017, 55, 1869-1877.	1.5	13
4	APINetworks Java. A Java approach to the efficient treatment of large-scale complex networks. <i>Computer Physics Communications</i> , 2016, 207, 549-552.	7.5	2
5	APINetworks: A general API for the treatment of complex networks in arbitrary computational environments. <i>Computer Physics Communications</i> , 2015, 196, 446-454.	7.5	2
6	Quantitative modeling of degree-degree correlation in complex networks. <i>Physical Review E</i> , 2013, 88, 032805.	2.1	3
7	A Survey of Parallel Programming Models and Tools in the Multi and Many-Core Era. <i>IEEE Transactions on Parallel and Distributed Systems</i> , 2012, 23, 1369-1386.	5.6	189
8	Analysis of the nitrile and methyl torsional vibrations of <i>n</i> -propyl cyanide in its $S_0$ electronic state. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3681-3694.	2.0	1
9	A uniform object-oriented solution to the eigenvalue problem for real symmetric and Hermitian matrices. <i>Computer Physics Communications</i> , 2011, 182, 2059-2064.	7.5	1
10	Structural and vibrational analysis of the OH torsional motion in difluorohydroxyborane. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 4389-4399.	2.0	1
11	A Concurrent Object-Oriented Approach to the Eigenproblem Treatment in Shared Memory Multicore Environments. <i>Lecture Notes in Computer Science</i> , 2011, , 630-642.	1.3	0
12	A general model for the generation and scheduling of parameter sweep experiments in computational grid environments. <i>Procedia Computer Science</i> , 2010, 1, 565-572.	2.0	0
13	Monitoring and steering Grid applications with GRID superscalar. <i>Future Generation Computer Systems</i> , 2010, 26, 645-653.	7.5	9
14	A metaheuristic approach to the optimal definition of molecule-fixed axes in rovibrational Hamiltonians. <i>Computer Physics Communications</i> , 2010, 181, 967-977.	7.5	2
15	Heuristic computation of the rovibrational G matrix in optimized molecule-fixed axes. <i>Gmat 2.1</i> . <i>Computer Physics Communications</i> , 2010, 181, 1471-1475.	7.5	3
16	Gmat. A software tool for the computation of the rovibrational G matrix. <i>Computer Physics Communications</i> , 2009, 180, 1183-1187.	7.5	6
17	Derivation of self-scheduling algorithms for heterogeneous distributed computer systems: Application to internet-based grids of computers. <i>Future Generation Computer Systems</i> , 2009, 25, 617-626.	7.5	16
18	A Fault Tolerant Adaptive Method for the Scheduling of Tasks in Dynamic Grids. , 2009, , .		2

#	ARTICLE	IF	CITATIONS
19	Structural and vibrational theoretical analysis of protonated formaldehyde in its $A^{\prime}$ ground electronic state. Theoretical Chemistry Accounts, 2008, 119, 343-354.	1.4	8
20	Accurate Numerical Computation of Rovibrational G Matrices in Molecules of Arbitrary Size. Lecture Notes in Computer Science, 2008, , 1011-1025.	1.3	1
21	A Heuristic Approach to Task Scheduling in Internet-Based Grids of Computers. , 2008, , .		1
22	MSSML: A Molecular Spectroscopic Simulations Markup Language for Rovibrational Studies. Lecture Notes in Computer Science, 2008, , 997-1010.	1.3	0
23	Performance of computationally intensive parameter sweep applications on Internet-based Grids of computers: the mapping of molecular potential energy hypersurfaces. Concurrency Computation Practice and Experience, 2007, 19, 463-481.	2.2	8
24	Molecular docking study of the binding of aminopyridines within the K <sup>+</sup> channel. Journal of Molecular Modeling, 2007, 13, 579-586.	1.8	26
25	A Quadratic Self-Scheduling Algorithm for Heterogeneous Distributed Computing Systems. , 2006, , .		3
26	Theoretical prediction of relative and absolute pKa values of aminopyridines. Biophysical Chemistry, 2006, 124, 155-160.	2.8	38
27	Customizing clustering computing for a computational chemistry environment. The case of the DBO-83 nicotinic analgesic. Computational and Theoretical Chemistry, 2005, 727, 41-48.	1.5	5
28	Conformational population distribution of acetylcholine, nicotine and muscarine in vacuum and solution. Computational and Theoretical Chemistry, 2005, 726, 115-124.	1.5	21
29	Theoretical Analysis of Pyridine Protonation in Water Clusters of Increasing Size. ChemPhysChem, 2005, 6, 139-147.	2.1	19
30	Analysis of B3LYP and MP2 conformational population distributions intrans-nicotine, acetylcholine, and ABT-594. International Journal of Quantum Chemistry, 2005, 103, 25-33.	2.0	13
31	Mechanism of Pyridine Protonation in Water Clusters of Increasing Size. Journal of Physical Chemistry A, 2005, 109, 8341-8347.	2.5	32
32	Thermodynamic conformational analysis and structural stability of the nicotinic analgesic ABT-594. Journal of Computer-Aided Molecular Design, 2003, 17, 713-724.	2.9	4
33	Rational modelling of the voltage-dependent K <sup>+</sup> channel inactivation by aminopyridines. Biophysical Chemistry, 2003, 104, 417-427.	2.8	20
34	Experimental and Theoretical Study of the Secondary Equilibrium Isotope Effect (SEIE) in the Proton Transfer between the Pyridinium-d <sub>5</sub> Cation and Pyridine. Journal of Physical Chemistry A, 2003, 107, 6160-6167.	2.5	8
35	Effect of the Conformational Kinetic Energy and the Rotovibrational Coupling in the Conformational Population of Bioactive Compounds. Journal of Physical Chemistry A, 2003, 107, 10191-10198.	2.5	7
36	Deprotonation Sites of Acetohydroxamic Acid Isomers. A Theoretical and Experimental Study. Journal of Organic Chemistry, 2003, 68, 6535-6542.	3.2	47

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37	Theoretical Study of the Effect of Hydrogen-Bonding on the Stability and Vibrational Spectrum of Isolated 2,2,2-Trifluoroethanol and Its Molecular Complexes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10673-10680.	2.5	34
38	The nature of the receptor site for the reversible K <sup>+</sup> channel blocking by aminopyridines. <i>Biophysical Chemistry</i> , 2002, 96, 1-14.	2.8	31
39	A computer simulation of the ring puckering and oxygen wagging dynamics in the S <sub>0</sub> state of cyclobutanone. <i>Advances in Quantum Chemistry</i> , 2001, 40, 345-359.	0.8	0
40	Theoretical analysis of the molecular determinants responsible for the K <sup>+</sup> channel blocking by aminopyridines. <i>Biophysical Chemistry</i> , 2001, 91, 49-60.	2.8	31
41	Large Amplitude Motions in Electronically Excited States: A Study of the S <sub>1</sub> Excited State of Formic Acid. <i>Progress in Theoretical Chemistry and Physics</i> , 2001, , 347-358.	0.2	0
42	Theoretical and Experimental Study of the Acetohydroxamic Acid Protonation: The Solvent Effect. <i>Chemistry - A European Journal</i> , 2000, 6, 2644-2652.	3.3	13
43	Suitability of different levels of theory for modelling of hydroxamic acids. <i>Computational and Theoretical Chemistry</i> , 2000, 530, 291-300.	1.5	15
44	Modeling of Protonation Processes in Acetohydroxamic Acid. <i>Journal of Organic Chemistry</i> , 2000, 65, 405-410.	3.2	114
45	The Torsion-Inversion Bending Energy Levels in the S <sub>1</sub> (n, $\tilde{\nu}^*$ ) Electronic State of Acetaldehyde. <i>Journal of Molecular Spectroscopy</i> , 1998, 190, 78-90.	1.2	12
46	Neural modeling of torsional potential hypersurfaces in non-rigid molecules. <i>Computers &amp; Chemistry</i> , 1998, 22, 355-361.	1.2	7
47	Effect of Large-Amplitude Vibrations on the Thermodynamics of Malondialdehyde. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1177-1180.	2.5	7
48	Enhanced procedure for the refinement of kinetic and potential functions for large-amplitude vibrations. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997, 93, 2989-2990.	1.7	0
49	Effect of Anharmonicities on the Thermodynamic Properties of the Water Dimer. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4128-4135.	2.5	41
50	The accurate computation of partition functions in non-rigid molecules. <i>Computers &amp; Chemistry</i> , 1997, 21, 143-151.	1.2	5
51	Theoretical study of the effect of torsional anharmonicity on the thermodynamic properties of methanol. <i>Chemical Physics Letters</i> , 1997, 273, 135-140.	2.6	30
52	The T <sub>1</sub> (n $\tilde{\nu}^*$ ) $\rightarrow$ S <sub>0</sub> laser induced phosphorescence excitation spectrum of acetaldehyde in a supersonic free jet: Torsion and wagging potentials in the lowest triplet state. <i>Journal of Chemical Physics</i> , 1996, 105, 2547-2552.	3.0	33
53	The Torsion-Inversion Energy Levels in the S <sub>1</sub> (n, $\tilde{\nu}^*$ ) Electronic State of Acetaldehyde from High-Resolution Jet-Cooled Fluorescence Excitation Spectroscopy. <i>Journal of Molecular Spectroscopy</i> , 1996, 175, 172-189.	1.2	21
54	Definition of a periodic methyl torsional coordinate in the S <sub>0</sub> state of acetaldehyde. <i>Journal of Molecular Structure</i> , 1995, 350, 83-89.	3.6	10

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55	Recursive computation of Hamiltonian matrix elements using harmonic oscillator eigenfunctions: Application to the inversion of ammonia and to the methyl torsion + aldehydic hydrogen wagging of acetaldehyde. <i>Computers &amp; Chemistry</i> , 1995, 19, 371-378.	1.2	18
56	Three-Dimensional Vibrational Study of the Coupling between Methyl Torsion and the Molecular Frame in the S <sub>0</sub> State of Acetaldehyde. <i>The Journal of Physical Chemistry</i> , 1995, 99, 8510-8515.	2.9	15
57	Derivation of accurate kinetic and potential-energy functions for several simultaneous large-amplitude vibrations: application to acetaldehyde in the S <sub>0</sub> and T <sub>1</sub> states. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1995, 91, 399-403.	1.7	16
58	Theoretical analysis of the structural and chemical reactivity properties of the schistosomicidal drug niridazole. <i>Journal De Chimie Physique Et De Physico-Chimie Biologique</i> , 1995, 92, 679-698.	0.2	0
59	On the origin of the barriers and the structures of acetaldehyde in its ground and first singlet excited state. <i>Theoretica Chimica Acta</i> , 1994, 88, 299-310.	0.8	13
60	Theoretical determination of the torsion-wagging structure of the S <sub>1</sub> $\hat{\rightarrow}$ S <sub>0</sub> electronic spectrum of acetaldehyde. <i>Chemical Physics</i> , 1994, 186, 221-231.	1.9	19
61	Computation of kinetic constants for large range internal motions in molecules. <i>Computers &amp; Chemistry</i> , 1994, 18, 27-32.	1.2	35
62	Vibrational energy levels and vibronic structure of electronic spectra in molecules with large amplitude motions. <i>Computers &amp; Chemistry</i> , 1994, 18, 413-417.	1.2	12
63	A study of quadratic + gaussian + cosine functions for the simultaneous description of intramolecular torsion and inversion. <i>Journal of Molecular Structure</i> , 1994, 318, 237-242.	3.6	11
64	A structural ab initio study of the T <sub>1</sub> triplet state of acetaldehyde. The effects of electron correlation and additional functions in the basis set. <i>Computational and Theoretical Chemistry</i> , 1994, 315, 9-17.	1.5	4
65	Wagging and torsion vibronic structure in the T <sub>1</sub> $\rightarrow$ S <sub>0</sub> electronic spectrum of acetaldehyde. <i>The Journal of Physical Chemistry</i> , 1994, 98, 1519-1524.	2.9	44
66	Quantum Mechanical Study and Nuclear Magnetic Resonance Measurements of Some $\hat{\pm}$ -Arylcarboxyalkyl Acids as Anti-inflammatory Agents. <i>Journal of Pharmaceutical Sciences</i> , 1989, 78, 764-766.	3.3	6
67	Étude comparative CNDO/2 des déterminants moléculaires de l'activité agoniste de récepteur-H <sub>2</sub> dans l'histamine et le bétazol. <i>European Journal of Medicinal Chemistry</i> , 1989, 24, 411-414.	5.5	4