

Sergio MartÃ-

List of Publications by Year in descending order

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80
papers

2,275
citations

185998

28
h-index

243296

44
g-index

82
all docs

82
docs citations

82
times ranked

1912
citing authors

#	ARTICLE	IF	CITATIONS
1	Theoretical insights in enzyme catalysis. <i>Chemical Society Reviews</i> , 2004, 33, 98-107.	18.7	150
2	Improving the QM/MM Description of Chemical Processes: A Dual Level Strategy To Explore the Potential Energy Surface in Very Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1008-1016.	2.3	120
3	Hybrid QM/MM Potentials of Mean Force with Interpolated Corrections. <i>Journal of Physical Chemistry B</i> , 2004, 108, 8427-8433.	1.2	95
4	A Hybrid Potential Reaction Path and Free Energy Study of the Chorismate Mutase Reaction. <i>Journal of the American Chemical Society</i> , 2001, 123, 1709-1712.	6.6	92
5	Theoretical Modeling of Enzyme Catalytic Power: Analysis of Cratic and Electrostatic Factors in CatecholO-Methyltransferase. <i>Journal of the American Chemical Society</i> , 2003, 125, 7726-7737.	6.6	79
6	Temperature Dependence of the Kinetic Isotope Effects in Thymidylate Synthase. A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2011, 133, 6692-6702.	6.6	60
7	Preorganization and Reorganization as Related Factors in Enzyme Catalysis: The Chorismate Mutase Case. <i>Chemistry - A European Journal</i> , 2003, 9, 984-991.	1.7	57
8	Hybrid Quantum Mechanics/Molecular Mechanics Simulations with Two-Dimensional Interpolated Corrections: Application to Enzymatic Processes. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17663-17670.	1.2	57
9	Increased Dynamic Effects in a Catalytically Compromised Variant of <i>Escherichia coli</i> Dihydrofolate Reductase. <i>Journal of the American Chemical Society</i> , 2013, 135, 18689-18696.	6.6	56
10	A QM/MM Study of the Conformational Equilibria in the Chorismate Mutase Active Site. The Role of the Enzymatic Deformation Energy Contribution. <i>Journal of Physical Chemistry B</i> , 2000, 104, 11308-11315.	1.2	54
11	A Theoretical Analysis of Rate Constants and Kinetic Isotope Effects Corresponding to Different Reactant Valleys in Lactate Dehydrogenase. <i>Journal of the American Chemical Society</i> , 2006, 128, 16851-16863.	6.6	52
12	Studying the role of protein dynamics in an SN2 enzyme reaction using free-energy surfaces and solvent coordinates. <i>Nature Chemistry</i> , 2013, 5, 566-571.	6.6	49
13	Protein Conformational Landscapes and Catalysis. Influence of Active Site Conformations in the Reaction Catalyzed by L-Lactate Dehydrogenase. <i>ACS Catalysis</i> , 2015, 5, 1172-1185.	5.5	48
14	A Theoretical Study of the Catalytic Mechanism of Formate Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10012-10022.	1.2	46
15	A Comparative Study of Claisen and Cope Rearrangements Catalyzed by Chorismate Mutase. An Insight into Enzymatic Efficiency: A Transition State Stabilization or Substrate Preorganization?. <i>Journal of the American Chemical Society</i> , 2004, 126, 311-319.	6.6	45
16	Transition structure selectivity in enzyme catalysis: a QM/MM study of chorismate mutase. <i>Theoretical Chemistry Accounts</i> , 2001, 105, 207-212.	0.5	44
17	Multipoint molecular recognition within a calix[6]arene funnel complex. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 10449-10454.	3.3	43
18	Computational design of biological catalyts. <i>Chemical Society Reviews</i> , 2008, 37, 2634.	18.7	41

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19	Theoretical Modeling of the Reaction Mechanism of Phosphate Monoester Hydrolysis in Alkaline Phosphatase. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7816-7824.	1.2	41
20	A Quantum Mechanics/Molecular Mechanics Study of the Protein-Ligand Interaction for Inhibitors of HIV-1 Integrase. <i>Chemistry - A European Journal</i> , 2007, 13, 7715-7724.	1.7	38
21	A Quantum Mechanics/Molecular Mechanics Study of the Catalytic Mechanism of the Thymidylate Synthase. <i>Biochemistry</i> , 2007, 46, 3704-3713.	1.2	35
22	Peptide Bond Formation Mechanism Catalyzed by Ribosome. <i>Journal of the American Chemical Society</i> , 2015, 137, 12024-12034.	6.6	34
23	Long Distance Electron-Transfer Mechanism in Peptidylglycine β -Hydroxylating Monooxygenase: A Perfect Fitting for a Water Bridge. <i>Journal of the American Chemical Society</i> , 2007, 129, 11700-11707.	6.6	33
24	Origin of the Absorption Maxima of the Photoactive Yellow Protein Resolved via Ab Initio Multiconfigurational Methods. <i>Journal of Physical Chemistry B</i> , 2008, 112, 7153-7156.	1.2	31
25	QM/MM Study of Thymidylate Synthase: Enzymatic Motions and the Temperature Dependence of the Rate Limiting Step. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2176-2182.	1.1	31
26	Theoretical Study of Primary Reaction of Pseudozyma antarctica Lipase B as the Starting Point To Understand Its Promiscuity. <i>ACS Catalysis</i> , 2014, 4, 426-434.	5.5	31
27	Toward Understanding the Photochemistry of Photoactive Yellow Protein: A CASPT2/CASSCF and Quantum Theory of Atoms in Molecules Combined Study of a Model Chromophore in Vacuo. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 3032-3038.	2.3	30
28	A QM/MM study of the complexes formed by aluminum and iron with serum transferrin at neutral and acidic pH. <i>Journal of Inorganic Biochemistry</i> , 2011, 105, 1446-1456.	1.5	30
29	The catalytic mechanism of glyceraldehyde 3-phosphate dehydrogenase from Trypanosoma cruzi elucidated via the QM/MM approach. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3772.	1.3	30
30	Computing Kinetic Isotope Effects for Chorismate Mutase with High Accuracy. A New DFT/MM Strategy. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3707-3710.	1.2	29
31	QM/MM calculations of kinetic isotope effects in the chorismate mutase active site. <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 483-487.	1.5	28
32	Vibrational analysis of the chorismate rearrangement: relaxed force constants, isotope effects and activation entropies calculated for reaction in vacuum, water and the active site of chorismate mutase. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 592-601.	0.9	28
33	Mechanism and Plasticity of Isochorismate Pyruvate Lyase: A Computational Study. <i>Journal of the American Chemical Society</i> , 2009, 131, 16156-16161.	6.6	28
34	A Quantum Mechanics/Molecular Mechanics Study of the Protein-Ligand Interaction of Two Potent Inhibitors of Human O-GlcNAcase: PUGNAc and NAG-Thiazoline. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14260-14266.	1.2	27
35	Predicting an Improvement of Secondary Catalytic Activity of Promiscuous Isochorismate Pyruvate Lyase by Computational Design. <i>Journal of the American Chemical Society</i> , 2008, 130, 2894-2895.	6.6	25
36	Catalytic Mechanism of Dihydrofolate Reductase Enzyme. A Combined Quantum-Mechanical/Molecular-Mechanical Characterization of the N5 Protonation Step. <i>Journal of Physical Chemistry B</i> , 2003, 107, 14036-14041.	1.2	24

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37	Computer-Aided Rational Design of Catalytic Antibodies: The 1F7 Case. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 286-290.	7.2	24
38	Analysis of the Decarboxylation Step in Mammalian Histidine Decarboxylase. <i>Journal of Biological Chemistry</i> , 2008, 283, 12393-12401.	1.6	24
39	Enzyme Molecular Mechanism as a Starting Point to Design New Inhibitors: A Theoretical Study of <i>α</i> -GlcNAcase. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6764-6775.	1.2	24
40	Theoretical studies of HIV-1 reverse transcriptase inhibition. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12614.	1.3	24
41	A Quantum Mechanic/Molecular Mechanic Study of the Wild-Type and N155S Mutant HIV-1 Integrase Complexed with Diketo Acid. <i>Biophysical Journal</i> , 2008, 94, 2443-2451.	0.2	23
42	Role of Solvent on Nonenzymatic Peptide Bond Formation Mechanisms and Kinetic Isotope Effects. <i>Journal of the American Chemical Society</i> , 2013, 135, 8708-8719.	6.6	23
43	A Collective Coordinate to Obtain Free Energy Profiles for Complex Reactions in Condensed Phases. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1795-1801.	2.3	20
44	Hybrid Schemes Based on Quantum Mechanics/Molecular Mechanics Simulations. <i>Advances in Protein Chemistry and Structural Biology</i> , 2011, 85, 81-142.	1.0	19
45	Computational Analysis of Human OGA Structure in Complex with PUGNAc and NAG-Thiazoline Derivatives. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 2775-2783.	2.5	19
46	Quantum Mechanics/Molecular Mechanics Studies of the Mechanism of Falcipain-2 Inhibition by the Epoxysuccinate E64. <i>Biochemistry</i> , 2014, 53, 3336-3346.	1.2	18
47	Calculation of binding energy using BLYP/MM for the HIV-1 integrase complexed with the S-1360 and two analogues. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 3818-3824.	1.4	17
48	Application of Grote's Hynes Theory to the Reaction Catalyzed by Thymidylate Synthase. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13593-13600.	1.2	17
49	Joint Use of Bonding Evolution Theory and QM/MM Hybrid Method for Understanding the Hydrogen Abstraction Mechanism via Cytochrome P450 Aromatase. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1470-1480.	2.3	17
50	Impact of Warhead Modulations on the Covalent Inhibition of SARS-CoV-2 M ^{pro} Explored by QM/MM Simulations. <i>ACS Catalysis</i> , 2022, 12, 698-708.	5.5	17
51	Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation of Wild-Type and Seven Mutants of <i>Cp</i> NagI in Complex with PUGNAc. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7029-7036.	1.2	16
52	Understanding the different activities of highly promiscuous MbtI by computational methods. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 3482.	1.3	16
53	QM/MM Theoretical Studies of a de Novo Retro-Aldolase Design. <i>ACS Catalysis</i> , 2019, 9, 2482-2492.	5.5	16
54	An AM1 theoretical study on the effect of Zn ²⁺ Lewis acid catalysis on the mechanism of the cycloaddition between 3-phenyl-1-(2-pyridyl)-2-propen-1-one and cyclopentadiene. <i>Tetrahedron</i> , 2002, 58, 2695-2700.	1.0	15

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55	Theoretical study of the temperature dependence of dynamic effects in thymidylate synthase. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11657.	1.3	15
56	Conformational equilibrium of chorismate. A QM/MM theoretical study combining statistical simulations and geometry optimisations in gas phase and in aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2003, 632, 197-206.	1.5	13
57	The effect of MM polarization on the QM/MM transition state stabilization: application to chorismate mutase. <i>Molecular Physics</i> , 2008, 106, 1511-1515.	0.8	13
58	Electrostatic effects in enzyme catalysis: a quantum mechanics/molecular mechanics study of the nucleophilic substitution reaction in haloalkane dehalogenase. <i>Theoretical Chemistry Accounts</i> , 2004, 112, 327.	0.5	11
59	A Novel Strategy to Study Electrostatic Effects in Chemical Reactions: Differences between the Role of Solvent and the Active Site of Chalcone Isomerase in a Michael Addition. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1532-1535.	2.3	10
60	Theoretical Studies on Mechanism of Inactivation of Kanamycin A by 4 th -O-Nucleotidyltransferase. <i>Frontiers in Chemistry</i> , 2018, 6, 660.	1.8	10
61	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 904-909.	7.2	9
62	Improving the QM/MM Description of Chemical Processes: A Dual Level Strategy To Explore the Potential Energy Surface in Very Large Systems. [<i>J. Chem. Theory Comput.</i> 1, 1008 ² , 1016 (2005)]. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 216-216.	2.3	9
63	Theoretical Study of Catalytic Efficiency of a Diels-Alderase Catalytic Antibody: An Indirect Effect Produced During the Maturation Process. <i>Chemistry - A European Journal</i> , 2008, 14, 596-602.	1.7	9
64	Theoretical QM/MM studies of enzymatic pericyclic reactions. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2010, 2, 115-131.	2.2	8
65	Molecular mechanism of chorismate mutase activity of promiscuous MbtI. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 601-607.	0.5	8
66	Do zwitterionic species exist in the non-enzymatic peptide bond formation?. <i>Chemical Communications</i> , 2012, 48, 11253.	2.2	8
67	QM/MM modeling of the hydroxylation of the androstenedione substrate catalyzed by cytochrome P450 aromatase (CYP19A1). <i>Journal of Computational Chemistry</i> , 2015, 36, 1736-1747.	1.5	8
68	QMCube (QM ³): An all-purpose suite for multiscale QM/MM calculations. <i>Journal of Computational Chemistry</i> , 2021, 42, 447-457.	1.5	8
69	Computational study of the mechanism of half-reactions in class 1A dihydroorotate dehydrogenase from <i>Trypanosoma cruzi</i> . <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18863.	1.3	7
70	Are Heme-Dependent Enzymes Always Using a Redox Mechanism? A Theoretical Study of the Kemp Elimination Catalyzed by a Promiscuous Aldoxime Dehydratase. <i>ACS Catalysis</i> , 2020, 10, 11110-11119.	5.5	7
71	Molecular mechanism of the site-specific self-cleavage of the RNA phosphodiester backbone by a twister ribozyme. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	6
72	Understanding the Directed Evolution of De Novo Retro-Aldolases from QM/MM Studies. <i>ACS Catalysis</i> , 2020, 10, 7871-7883.	5.5	6

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73	Theoretical Study of the Mechanism of Exemestane Hydroxylation Catalyzed by Human Aromatase Enzyme. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3331-3343.	1.2	5
74	Unrevealing the Proteolytic Activity of RgpB Gingipain from Computational Simulations. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4582-4593.	2.5	4
75	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. <i>Angewandte Chemie</i> , 2005, 117, 926-931.	1.6	3
76	Stereoselectivity Behavior of the AZ28 Antibody Catalyzed Oxy-Cope Rearrangement. <i>Journal of Physical Chemistry A</i> , 2006, 110, 726-730.	1.1	3
77	New insight into the electronic structure of iron(IV)oxo porphyrin compound I. A quantum chemical topological analysis. <i>Journal of Computational Chemistry</i> , 2013, 34, 780-789.	1.5	3
78	Examination of the performance of semiempirical methods in QM/MM studies of the SN2-like reaction of an adenylyl group transfer catalysed by ANT4. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	1
79	A QM/MM study on the origin of retro-aldolase activity of a catalytic antibody. <i>Chemical Communications</i> , 2021, 57, 5306-5309.	2.2	0
80	Computational Modeling of Biological Systems: The LDH Story. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2010, , 355-374.	0.6	0