

Mireia Garcia-Viloca

List of Publications by Year in descending order

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48
papers

3,375
citations

185998

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h-index

205818

48
g-index

49
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docs citations

49
times ranked

2684
citing authors

#	ARTICLE	IF	CITATIONS
1	Understanding how cAMP-dependent protein kinase can catalyze phosphoryl transfer in the presence of Ca ²⁺ and Sr ²⁺ : a QM/MM study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10377-10394.	1.3	6
2	A QM/MM study of Kemptide phosphorylation catalyzed by protein kinase A. The role of Asp166 as a general acid/base catalyst. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 3497-3511.	1.3	18
3	SP20 Phosphorylation Reaction Catalyzed by Protein Kinase A: QM/MM Calculations Based on Recently Determined Crystallographic Structures. <i>ACS Catalysis</i> , 2015, 5, 4897-4912.	5.5	19
4	A QM/MM study of the associative mechanism for the phosphorylation reaction catalyzed by protein kinase A and its D166A mutant. <i>Journal of Computer-Aided Molecular Design</i> , 2014, 28, 1077-1091.	1.3	11
5	Theoretical Analysis of the Catalytic Mechanism of <i>Helicobacter pylori</i> Glutamate Racemase. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12406-12414.	1.2	12
6	Theoretical Study of the Mechanism of the Hydride Transfer between Ferredoxin-NADP ⁺ Reductase and NADP ⁺ : The Role of Tyr303. <i>Journal of the American Chemical Society</i> , 2012, 134, 20544-20553.	6.6	40
7	Influence of the enzyme phosphorylation state and the substrate on PKA enzyme dynamics. <i>Biophysical Chemistry</i> , 2012, 161, 17-28.	1.5	9
8	A QM/MM study of the phosphoryl transfer to the Kemptide substrate catalyzed by protein kinase A. The effect of the phosphorylation state of the protein on the mechanism. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 530-539.	1.3	25
9	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
10	Mechanism of the Hydride Transfer between <i>Anabaena</i> Tyr303Ser FNR _{rd} /FNR _{ox} and NADP ⁺ /H. A Combined Pre-Steady-State Kinetic/Ensemble-Averaged Transition-State Theory with Multidimensional Tunneling Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 3368-3379.	1.2	27
11	Benchmark calculations on models of the phosphoryl transfer reaction catalyzed by protein kinase A. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 197-215.	0.5	4
12	How the Substrate d-Glutamate Drives the Catalytic Action of <i>Bacillus subtilis</i> Glutamate Racemase. <i>Journal of the American Chemical Society</i> , 2009, 131, 3509-3521.	6.6	23
13	Critical Role of Substrate Conformational Change in the Proton Transfer Process Catalyzed by 4-Oxalocrotonate Tautomerase. <i>Journal of the American Chemical Society</i> , 2009, 131, 2687-2698.	6.6	18
14	New Insights into the Reaction Mechanism Catalyzed by the Glutamate Racemase Enzyme: A pH Titration Curves and Classical Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2385-2397.	1.2	13
15	Comparative study of the prereactive protein kinase A Michaelis complex with Kemptide substrate. <i>Journal of Computer-Aided Molecular Design</i> , 2007, 21, 603-615.	1.3	7
16	Enzyme Dynamics and Tunneling Enhanced by Compression in the Hydrogen Abstraction Catalyzed by Soybean Lipoxygenase-1. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24708-24719.	1.2	51
17	On the Ionization State of the Substrate in the Active Site of Glutamate Racemase. A QM/MM Study about the Importance of Being Zwitterionic. <i>Journal of Physical Chemistry A</i> , 2006, 110, 717-725.	1.1	33
18	Path Integral Simulations of Proton Transfer Reactions in Aqueous Solution Using Combined QM/MM Potentials. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 236-245.	2.3	57

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19	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
20	A Molecular Dynamics Simulation of the Binding Modes of d-Glutamate and d-Glutamine to Glutamate Racemase. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 737-749.	2.3	9
21	A QM/MM Exploration of the Potential Energy Surface of Pyruvate to Lactate Transformation Catalyzed by LDH. Improving the Accuracy of Semiempirical Descriptions. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 750-761.	2.3	22
22	Nonperfect Synchronization of Reaction Center Rehybridization in the Transition State of the Hydride Transfer Catalyzed by Dihydrofolate Reductase. <i>Journal of the American Chemical Society</i> , 2005, 127, 14879-14886.	6.6	56
23	Solvent and Protein Effects on the Vibrational Frequency Shift and Energy Relaxation of the Azide Ligand in Carbonic Anhydrase. <i>Journal of Physical Chemistry B</i> , 2004, 108, 13501-13512.	1.2	34
24	Sensitivity of molecular dynamics simulations to the choice of the X-ray structure used to model an enzymatic reaction. <i>Protein Science</i> , 2004, 13, 2341-2354.	3.1	32
25	Generalized hybrid orbital for the treatment of boundary atoms in combined quantum mechanical and molecular mechanical calculations using the semiempirical parameterized model 3 method. <i>Theoretical Chemistry Accounts</i> , 2004, 111, 280-286.	0.5	35
26	Ensemble-averaged variational transition state theory with optimized multidimensional tunneling for enzyme kinetics and other condensed-phase reactions. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 1136-1152.	1.0	122
27	Dynamics of an Enzymatic Substitution Reaction in Haloalkane Dehalogenase. <i>Journal of the American Chemical Society</i> , 2004, 126, 1369-1376.	6.6	68
28	How Enzymes Work: Analysis by Modern Rate Theory and Computer Simulations. <i>Science</i> , 2004, 303, 186-195.	6.0	1,048
29	Semiempirical QM/MM potential with simple valence bond (SVB) for enzyme reactions. Application to the nucleophilic addition reaction in haloalkane dehalogenase. <i>Theoretical Chemistry Accounts</i> , 2003, 109, 133-139.	0.5	33
30	Hydride transfer catalyzed by xylose isomerase: Mechanism and quantum effects. <i>Journal of Computational Chemistry</i> , 2003, 24, 177-190.	1.5	90
31	Free Energy Surface, Reaction Paths, and Kinetic Isotope Effect of Short-Chain Acyl-CoA Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2003, 107, 9567-9578.	1.2	75
32	Reaction-Path Energetics and Kinetics of the Hydride Transfer Reaction Catalyzed by Dihydrofolate Reductase. <i>Biochemistry</i> , 2003, 42, 13558-13575.	1.2	202
33	Solvent effects, reaction coordinates, and reorganization energies on nucleophilic substitution reactions in aqueous solution. <i>Advances in Physical Organic Chemistry</i> , 2003, 38, 161-181.	0.5	10
34	Importance of Substrate and Cofactor Polarization in the Active Site of Dihydrofolate Reductase. <i>Journal of Molecular Biology</i> , 2003, 327, 549-560.	2.0	78
35	The Incorporation of Quantum Effects in Enzyme Kinetics Modeling. <i>Accounts of Chemical Research</i> , 2002, 35, 341-349.	7.6	240
36	Quantum Dynamics of Hydride Transfer Catalyzed by Bimetallic Electrophilic Catalysis: Synchronous Motion of Mg ²⁺ and H ⁻ in Xylose Isomerase. <i>Journal of the American Chemical Society</i> , 2002, 124, 7268-7269.	6.6	35

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37	On the modulation of the substrate activity for the racemization catalyzed by mandelate racemase enzyme. A QM/MM study. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 5365-5371.	1.3	9
38	The search for stationary points on a quantum mechanical/molecular mechanical potential-energy surface. <i>Theoretical Chemistry Accounts</i> , 2002, 107, 147-153.	0.5	16
39	The ¹ H NMR Chemical Shift for the Hydroxy Proton of 4-(Dimethylamino)-2-hydroxychalcone in Chloroform: A Theoretical Approach to Its Inverse Dependence on the Temperature. <i>Organic Letters</i> , 2001, 3, 589-592.	2.4	11
40	A QM/MM Study of the Racemization of Vinylglycolate Catalyzed by Mandelate Racemase Enzyme. <i>Journal of the American Chemical Society</i> , 2001, 123, 709-721.	6.6	38
41	Canonical Variational Theory for Enzyme Kinetics with the Protein Mean Force and Multidimensional Quantum Mechanical Tunneling Dynamics. Theory and Application to Liver Alcohol Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2001, 105, 11326-11340.	1.2	184
42	Inclusion of quantum-mechanical vibrational energy in reactive potentials of mean force. <i>Journal of Chemical Physics</i> , 2001, 114, 9953-9958.	1.2	84
43	Molecular dynamics simulations can reproduce the subtle differences in NADP and NHDP binding to isocitrate dehydrogenase. <i>International Journal of Quantum Chemistry</i> , 1999, 75, 231-243.	1.0	1
44	Asymmetry of the Hydrogen Bond of Hydrogen Phthalate Anion in Solution. A QM/MM Study. <i>Journal of the American Chemical Society</i> , 1999, 121, 9198-9207.	6.6	51
45	Temperature Dependence of Proton NMR Chemical Shift As a Criterion To Identify Low-Barrier Hydrogen Bonds. <i>Journal of the American Chemical Society</i> , 1998, 120, 10203-10209.	6.6	53
46	Is an Extremely Low-Field Proton Signal in the NMR Spectrum Conclusive Evidence for a Low-Barrier Hydrogen Bond?. <i>Journal of Physical Chemistry A</i> , 1997, 101, 8727-8733.	1.1	55
47	On pKa Matching as a Requirement To Form a Low-Barrier Hydrogen Bond. A Theoretical Study in Gas Phase. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3880-3886.	1.1	48
48	Theoretical Study of the Low-Barrier Hydrogen Bond in the Hydrogen Maleate Anion in the Gas Phase. Comparison with Normal Hydrogen Bonds. <i>Journal of the American Chemical Society</i> , 1997, 119, 1081-1086.	6.6	151