# Mireia Garcia-Viloca

List of Publications by Year
in descending order



| | | | |
|---|---|---|---|
| 48 papers | 3,375 citations | 186209 28 h-index | 206029 48 g-index |
| 49 all docs | 49 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 Ca2+and Sr2+: a QM/MM study. Physical Chemistry Chemical Physics, 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. Physical Chemistry Chemical Physics, 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. ACS Catalysis, 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. Journal of Computer-Aided Molecular Design, 2014, 28, 1077-1091. | 1.3 | 11 |
| 5 | Theoretical Analysis of the Catalytic Mechanism of Helicobacter pylori Glutamate Racemase. Journal of Physical Chemistry B, 2012, 116, 12406-12414. | 1.2 | 12 |
| 6 | Theoretical Study of the Mechanism of the Hydride Transfer between Ferredoxinâ€“NADP<sup>+</sup> Reductase and NADP<sup>+</sup>: The Role of Tyr303. Journal of the American Chemical Society, 2012, 134, 20544-20553. | 6.6 | 40 |
| 7 | Influence of the enzyme phosphorylation state and the substrate on PKA enzyme dynamics. Biophysical Chemistry, 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. Physical Chemistry Chemical Physics, 2011, 13, 530-539. | 1.3 | 25 |
| 9 | Temperature Dependence of the Kinetic Isotope Effects in Thymidylate Synthase. A Theoretical Study. Journal of the American Chemical Society, 2011, 133, 6692-6702. | 6.6 | 60 |
| 10 | Mechanism of the Hydride Transfer between Anabaena Tyr303Ser FNR<sub>rd</sub>/FNR<sub>ox</sub> and NADP<sup>+</sup>/H. A Combined Pre-Steady-State Kinetic/Ensemble-Averaged Transition-State Theory with Multidimensional Tunneling Study. Journal of Physical Chemistry B, 2010, 114, 3368-3379. | 1.2 | 27 |
| 11 | Benchmark calculations on models of the phosphoryl transfer reaction catalyzed by protein kinase A. Theoretical Chemistry Accounts, 2009, 124, 197-215. | 0.5 | 4 |
| 12 | How the Substrate d-Glutamate Drives the Catalytic Action of Bacillus subtilis Glutamate Racemase. Journal of the American Chemical Society, 2009, 131, 3509-3521. | 6.6 | 23 |
| 13 | Critical Role of Substrate Conformational Change in the Proton Transfer Process Catalyzed by 4-Oxalocrotonate Tautomerase. Journal of the American Chemical Society, 2009, 131, 2687-2698. | 6.6 | 18 |
| 14 | New Insights into the Reaction Mechanism Catalyzed by the Glutamate Racemase Enzyme:Â pH Titration Curves and Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 2385-2397. | 1.2 | 13 |
| 15 | Comparative study of the prereactive protein kinase A Michaelis complex with Kemptide substrate. Journal of Computer-Aided Molecular Design, 2007, 21, 603-615. | 1.3 | 7 |
| 16 | Enzyme Dynamics and Tunneling Enhanced by Compression in the Hydrogen Abstraction Catalyzed by Soybean Lipoxygenase-1. Journal of Physical Chemistry B, 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 Zwitterionicâ€. Journal of Physical Chemistry A, 2006, 110, 717-725. | 1.1 | 33 |
| 18 | Path Integral Simulations of Proton Transfer Reactions in Aqueous Solution Using Combined QM/MM Potentials. Journal of Chemical Theory and Computation, 2006, 2, 236-245. | 2.3 | 57 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | A Theoretical Analysis of Rate Constants and Kinetic Isotope Effects Corresponding to Different Reactant Valleys in Lactate Dehydrogenase. Journal of the American Chemical Society, 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. Journal of Chemical Theory and Computation, 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. Journal of Chemical Theory and Computation, 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. Journal of the American Chemical Society, 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. Journal of Physical Chemistry B, 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. Protein Science, 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. Theoretical Chemistry Accounts, 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. International Journal of Quantum Chemistry, 2004, 100, 1136-1152. | 1.0 | 122 |
| 27 | Dynamics of an Enzymatic Substitution Reaction in Haloalkane Dehalogenase. Journal of the American Chemical Society, 2004, 126, 1369-1376. | 6.6 | 68 |
| 28 | How Enzymes Work: Analysis by Modern Rate Theory and Computer Simulations. Science, 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. Theoretical Chemistry Accounts, 2003, 109, 133-139. | 0.5 | 33 |
| 30 | Hydride transfer catalyzed by xylose isomerase: Mechanism and quantum effects. Journal of Computational Chemistry, 2003, 24, 177-190. | 1.5 | 90 |
| 31 | Free Energy Surface, Reaction Paths, and Kinetic Isotope Effect of Short-Chain Acyl-CoA Dehydrogenase. Journal of Physical Chemistry B, 2003, 107, 9567-9578. | 1.2 | 75 |
| 32 | Reaction-Path Energetics and Kinetics of the Hydride Transfer Reaction Catalyzed by Dihydrofolate Reductase. Biochemistry, 2003, 42, 13558-13575. | 1.2 | 202 |
| 33 | Solvent effects, reaction coordinates, and reorganization energies on nucleophilic substitution reactions in aqueous solution. Advances in Physical Organic Chemistry, 2003, 38, 161-181. | 0.5 | 10 |
| 34 | Importance of Substrate and Cofactor Polarization in the Active Site of Dihydrofolate Reductase. Journal of Molecular Biology, 2003, 327, 549-560. | 2.0 | 78 |
| 35 | The Incorporation of Quantum Effects in Enzyme Kinetics Modeling. Accounts of Chemical Research, 2002, 35, 341-349. | 7.6 | 240 |
| 36 | Quantum Dynamics of Hydride Transfer Catalyzed by Bimetallic Electrophilic Catalysis:â€‰ Synchronous Motion of Mg2+ and H- in Xylose Isomerase. Journal of the American Chemical Society, 2002, 124, 7268-7269. | 6.6 | 35 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | On the modulation of the substrate activity for the racemization catalyzed by mandelate racemase enzyme. A QM/MM study. Physical Chemistry Chemical Physics, 2002, 4, 5365-5371. | 1.3 | 9 |
| 38 | The search for stationary points on a quantum mechanical/molecular mechanical potential-energy surface. Theoretical Chemistry Accounts, 2002, 107, 147-153. | 0.5 | 16 |
| 39 | The1H NMR Chemical Shift for the Hydroxy Proton of 4-(Dimethylamino)-2â€˜-hydroxychalcone in Chloroform:â€‰ A Theoretical Approach to Its Inverse Dependence on the Temperature. Organic Letters, 2001, 3, 589-592. | 2.4 | 11 |
| 40 | A QM/MM Study of the Racemization of Vinylglycolate Catalyzed by Mandelate Racemase Enzyme. Journal of the American Chemical Society, 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. Journal of Physical Chemistry B, 2001, 105, 11326-11340. | 1.2 | 184 |
| 42 | Inclusion of quantum-mechanical vibrational energy in reactive potentials of mean force. Journal of Chemical Physics, 2001, 114, 9953-9958. | 1.2 | 84 |
| 43 | Molecular dynamics simulations can reproduce the subtle differences in NADP and NHDP binding to isocitrate dehydrogenase. International Journal of Quantum Chemistry, 1999, 75, 231-243. | 1.0 | 1 |
| 44 | Asymmetry of the Hydrogen Bond of Hydrogen Phthalate Anion in Solution. A QM/MM Study. Journal of the American Chemical Society, 1999, 121, 9198-9207. | 6.6 | 51 |
| 45 | Temperature Dependence of Proton NMR Chemical Shift As a Criterion To Identify Low-Barrier Hydrogen Bonds. Journal of the American Chemical Society, 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?. Journal of Physical Chemistry A, 1997, 101, 8727-8733. | 1.1 | 55 |
| 47 | On pKaMatching as a Requirement To Form a Low-Barrier Hydrogen Bond. A Theoretical Study in Gas Phase. Journal of Physical Chemistry A, 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. Journal of the American Chemical Society, 1997, 119, 1081-1086. | 6.6 | 151 |