Massimo Delle Piane

List of Publications by Year
in descending order

20	518	758635 12	794141 19
papers	citations	h-index	g-index

20	20	20	800
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Can Mesoporous Silica Speed Up Degradation of Benzodiazepines? Hints from Quantum Mechanical Investigations. Materials, 2022, 15, 1357.	1.3	2
2	Lessons from a Challenging System: Accurate Adsorption Free Energies at the Amino Acid/ZnO Interface. Journal of Chemical Theory and Computation, 2021, 17, 4420-4434.	2.3	5
3	The puzzling issue of silica toxicity: are silanols bridging the gaps between surface states and pathogenicity?. Particle and Fibre Toxicology, 2019, 16, 32.	2.8	72
4	Impact of the Conformational Variability of Oligopeptides on the Computational Prediction of Their CD Spectra. Journal of Physical Chemistry B, 2019, 123, 6694-6704.	1.2	7
5	Ligand-functionalized Pt nanoparticles as asymmetric heterogeneous catalysts: molecular reaction control by ligandâ€“reactant interactions. Catalysis Science and Technology, 2018, 8, 6062-6075.	2.1	19
6	Atomistic Details of Chymotrypsin Conformational Changes upon Adsorption on Silica. ACS Biomaterials Science and Engineering, 2018, 4, 4036-4050.	2.6	15
7	Structural and Computational Assessment of the Influence of Wet-Chemical Post-Processing of the Al-Substituted Cubic Li₇La₃Zr₂O₁₂. ACS Applied Materials & Interfaces, 2018, 10, 37188-37197.	4.0	30
8	Ab Initio Modeling of Hydrogen Bond Interaction at Silica Surfaces With Focus on Silica/Drugs Systems. , 2018, , 297-328.		6
9	Molecular Dynamics Simulations of the Silicaâ€“Cell Membrane Interaction: Insights on Biomineralization and Nanotoxicity. Journal of Physical Chemistry C, 2018, 122, 21330-21343.	1.5	23
10	Models for biomedical interfaces: a computational study of quinone-functionalized amorphous silica surface features. Physical Chemistry Chemical Physics, 2017, 19, 7793-7806.	1.3	11
11	Propionic acid derivatives confined in mesoporous silica: monomers or dimers? The case of ibuprofen investigated by static and dynamic ab initio simulations. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	6
12	Elucidating the fundamental forces in protein crystal formation: the case of crambin. Chemical Science, 2016, 7, 1496-1507.	3.7	21
13	Water at hydroxyapatite surfaces: the effect of coverage and surface termination as investigated by all-electron B3LYP-D* simulations. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	29
14	Simulation and Experiment Reveal a Complex Scenario for the Adsorption of an Antifungal Drug in Ordered Mesoporous Silica. Journal of Physical Chemistry C, 2015, 119, 13068-13079.	1.5	27
15	Computational Study of Acidic and Basic Functionalized Crystalline Silica Surfaces as a Model for Biomaterial Interfaces. Langmuir, 2015, 31, 6321-6331.	1.6	11
16	CO₃^{2â€“} Mobility in Carbonate Apatite As Revealed by Density Functional Modeling. Journal of Physical Chemistry C, 2014, 118, 1364-1369.	1.5	20
17	Large-Scale B3LYP Simulations of Ibuprofen Adsorbed in MCM-41 Mesoporous Silica as Drug Delivery System. Journal of Physical Chemistry C, 2014, 118, 26737-26749.	1.5	52
18	Silica-Based Materials as Drug Adsorbents: First Principle Investigation on the Role of Water Microsolvation on Ibuprofen Adsorption. Journal of Physical Chemistry A, 2014, 118, 5801-5807.	1.1	47

#	Article	IF	Citations
19	Does Dispersion Dominate over H-Bonds in Drugâ€“Surface Interactions? The Case of Silica-Based Materials As Excipients and Drug-Delivery Agents. Journal of Chemical Theory and Computation, 2013, 9, 2404-2415.	2.3	72
20	A new massively parallel version of CRYSTAL for large systems on high performance computing architectures. Journal of Computational Chemistry, 2012, 33, 2276-2284.	1.5	43