# 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 | 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 |
| 2 | 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 |
| 3 | 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 |
| 4 | 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 |
| 5 | 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 |
| 6 | Structural and Computational Assessment of the Influence of Wet-Chemical Post-Processing of the Al-Substituted Cubic Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub>. ACS Applied Materials & Interfaces, 2018, 10, 37188-37197. | 4.0 | 30 |
| 7 | 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 |
| 8 | 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 |
| 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 | Elucidating the fundamental forces in protein crystal formation: the case of crambin. Chemical Science, 2016, 7, 1496-1507. | 3.7 | 21 |
| 11 | CO<sub>3</sub><sup>2â€“</sup> Mobility in Carbonate Apatite As Revealed by Density Functional Modeling. Journal of Physical Chemistry C, 2014, 118, 1364-1369. | 1.5 | 20 |
| 12 | 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 |
| 13 | Atomistic Details of Chymotrypsin Conformational Changes upon Adsorption on Silica. ACS Biomaterials Science and Engineering, 2018, 4, 4036-4050. | 2.6 | 15 |
| 14 | Computational Study of Acidic and Basic Functionalized Crystalline Silica Surfaces as a Model for Biomaterial Interfaces. Langmuir, 2015, 31, 6321-6331. | 1.6 | 11 |
| 15 | 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 |
| 16 | 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 |
| 17 | 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 |
| 18 | Ab Initio Modeling of Hydrogen Bond Interaction at Silica Surfaces With Focus on Silica/Drugs Systems. , 2018, , 297-328. | | 6 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | Can Mesoporous Silica Speed Up Degradation of Benzodiazepines? Hints from Quantum Mechanical Investigations. Materials, 2022, 15, 1357. | 1.3 | 2 |