Marta Corno

List of Publications by Year
in descending order

71 papers	2,061 citations	185998 28 h-index	253896 43 g-index
76 all docs	76 docs citations	76 times ranked	2162 citing authors

#	Article	IF	Citations
1	Water Interaction with Fe2NiP Schreibersite (110) Surface: a Quantum Mechanical Atomistic Perspective. Journal of Physical Chemistry C, 2022, 126, 2243-2252.	1.5	1
2	Can Mesoporous Silica Speed Up Degradation of Benzodiazepines? Hints from Quantum Mechanical Investigations. Materials, 2022, 15, 1357.	1.3	2
3	Molecular recognition between membrane epitopes and nearly free surface silanols explains silica membranolytic activity. Colloids and Surfaces B: Biointerfaces, 2022, 217, 112625.	2.5	16
4	Ab initio Calculation of Binding Energies of Interstellar Sulphur-Containing Species on Crystalline Water Ice Models. Lecture Notes in Computer Science, 2021, , 608-619.	1.0	1
5	Solid-State Conformational Flexibility at Work: Energetic Landscape of a Single Crystal-to-Single Crystal Transformation in a Cyclic Hexapeptoid. Crystal Growth and Design, 2021, 21, 897-907.	1.4	13
6	Computing Binding Energies of Interstellar Molecules by Semiempirical Quantum Methods: Comparison Between DFT and GFN2 on Crystalline Ice. Lecture Notes in Computer Science, 2021, , 632-645.	1.0	3
7	Simulation of nanosizing effects in the decomposition of Ca(BH4)2 through atomistic thin film models. Research on Chemical Intermediates, 2021, 47, 345-356.	1.3	7
8	Balancing Cost and Accuracy in Quantum Mechanical Simulations on Collagen Protein Models. Journal of Chemical Theory and Computation, 2021, 17, 2566-2574.	2.3	9
9	Ab Initio Computational Study on Fe2NiP Schreibersite: Bulk and Surface Characterization. ACS Earth and Space Chemistry, 2021, 5, 1741-1751.	1.2	6
10	Theoretical and Experimental Studies of LiBH₄â€“LiBr Phase Diagram. ACS Applied Energy Materials, 2021, 4, 7327-7337.	2.5	12
11	On the Interactions of Melatonin/Î²-Cyclodextrin Inclusion Complex: A Novel Approach Combining Efficient Semiempirical Extended Tight-Binding (xTB) Results with Ab Initio Methods. Molecules, 2021, 26, 5881.	1.7	16
12	Solid-State Hydrogen Storage Systems and the Relevance of a Gender Perspective. Energies, 2021, 14, 6158.	1.6	10
13	Computational Surface Modelling of Ices and Minerals of Interstellar Interestâ€”Insights and Perspectives. Minerals (Basel, Switzerland), 2021, 11, 26.	0.8	13
14	How Does Collagen Adsorb on Hydroxyapatite? Insights From Ab Initio Simulations on a Polyproline Type II Model. Journal of Physical Chemistry C, 2019, 123, 7540-7550.	1.5	31
15	Properties and Reactivity toward Water of A Type Carbonated Apatite and Hydroxyapatite Surfaces. Journal of Physical Chemistry C, 2018, 122, 3934-3944.	1.5	18
16	Ab Initio Modeling of Hydrogen Bond Interaction at Silica Surfaces With Focus on Silica/Drugs Systems. , 2018, , 297-328.		6
17	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
18	Method Dependence of Proline Ring Flexibility in the Poly-<scp>l</scp>-Proline Type II Polymer. Journal of Chemical Theory and Computation, 2017, 13, 370-379.	2.3	16

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19	How strong are H-bonds at the fully hydroxylated silica surfaces? Insights from the B3LYP electron density topological analysis. Structural Chemistry, 2017, 28, 1009-1015.	1.0	15
20	Phase diagrams of the LiBH₄â€“NaBH₄â€“KBH₄ system. Physical Chemistry Chemical Physics, 2017, 19, 25071-25079.	1.3	20
21	Forsterite Surfaces as Models of Interstellar Core Dust Grains: Computational Study of Carbon Monoxide Adsorption. ACS Earth and Space Chemistry, 2017, 1, 384-398.	1.2	21
22	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
23	Assessment of Different Quantum Mechanical Methods for the Prediction of Structure and Cohesive Energy of Molecular Crystals. Journal of Chemical Theory and Computation, 2016, 12, 3340-3352.	2.3	85
24	A thermodynamic investigation of the LiBH₄â€“NaBH₄ system. RSC Advances, 2016, 6, 60101-60108.	1.7	23
25	Elucidating the fundamental forces in protein crystal formation: the case of crambin. Chemical Science, 2016, 7, 1496-1507.	3.7	21
26	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
27	Surface Modeling of Ceramic Biomaterials. , 2016, , 3935-3947.		0
28	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
29	Computational Study of Acidic and Basic Functionalized Crystalline Silica Surfaces as a Model for Biomaterial Interfaces. Langmuir, 2015, 31, 6321-6331.	1.6	11
30	Surface Modeling of Ceramic Biomaterials. , 2015, , 1-13.		0
31	DFT investigation of structural and vibrational properties of type B and mixed A-B carbonated hydroxylapatite. American Mineralogist, 2014, 99, 117-127.	0.9	35
32	CO₃^{2â€“} Mobility in Carbonate Apatite As Revealed by Density Functional Modeling. Journal of Physical Chemistry C, 2014, 118, 1364-1369.	1.5	20
33	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
34	Halide substitution in Ca(BH₄)₂. RSC Advances, 2014, 4, 4736-4742.	1.7	22
35	Probing the fate of interstitial water in bulk bioactive glass by ab initio simulations. RSC Advances, 2014, 4, 36425-36436.	1.7	14
36	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

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37	Effects of metastability on hydrogen sorption in fluorine substituted hydrides. Journal of Alloys and Compounds, 2014, 615, S706-S710.	2.8	12
38	Revealing Hydroxyapatite Nanoparticle Surface Structure by CO Adsorption: A Combined B3LYP and Infrared Study. Journal of Physical Chemistry C, 2013, 117, 25526-25534.	1.5	18
39	Periodic ab initio bulk investigation of hydroxylapatite and type A carbonated apatite with both pseudopotential and all-electron basis sets for calcium atoms. American Mineralogist, 2013, 98, 410-416.	0.9	35
40	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
41	The vibrational features of hydroxylapatite and type A carbonated apatite: A first principle contribution. American Mineralogist, 2013, 98, 752-759.	0.9	55
42	DFT Modeling of 45S5 and 77S Soda-Lime Phospho-Silicate Glass Surfaces: Clues on Different Bioactivity Mechanism. Langmuir, 2013, 29, 5749-5759.	1.6	20
43	Thermodynamic Tuning of Calcium Hydride by Fluorine Substitution. Materials Research Society Symposia Proceedings, 2012, 1441, 17.	0.1	6
44	Ab initio modelling of proteinâ€“biomaterial interactions: influence of amino acid polar side chains on adsorption at hydroxyapatite surfaces. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 1478-1498.	1.6	30
45	Stability of the Dipolar (001) Surface of Hydroxyapatite. Journal of Physical Chemistry C, 2012, 116, 6108-6114.	1.5	36
46	Halide Substitution in Magnesium Borohydride. Journal of Physical Chemistry C, 2012, 116, 12482-12488.	1.5	35
47	Glycine Adsorption at Nonstoichiometric (010) Hydroxyapatite Surfaces: A B3LYP Study. Journal of Physical Chemistry C, 2012, 116, 14561-14567.	1.5	36
48	Synthesis and Structural Investigation of Zr(BH₄)₄. Journal of Physical Chemistry C, 2012, 116, 20239-20245.	1.5	43
49	Coordination chemistry of Ca sites at the surface of nanosized hydroxyapatite: interaction with H ₂ O and CO. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 1313-1336.	1.6	48
50	Theoretical and Experimental Study of LiBH4-LiCl Solid Solution. Crystals, 2012, 2, 144-158.	1.0	30
51	Vibrational Properties of MBH₄ and MBF₄ Crystals (M = Li, Na, K): A Combined DFT, Infrared, and Raman Study. Journal of Physical Chemistry C, 2011, 115, 18890-18900.	1.5	39
52	Experimental and computational investigations on the AlH3/AlF3 system. Journal of Alloys and Compounds, 2011, 509, 10-14.	2.8	19
53	A computational study on the effect of fluorine substitution in LiBH4. Journal of Alloys and Compounds, 2011, 509, S679-S683.	2.8	36
54	Affinity of hydroxyapatite (001) and (010) surfaces to formic and alendronic acids: a quantum-mechanical and infrared study. Physical Chemistry Chemical Physics, 2011, 13, 1099-1111.	1.3	27

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55	Probing vibrational modes in silica glass using inelastic neutron scattering with mass contrast. Physical Review B, 2010, 81, .	1.1	14
56	Hydroxyapatite as a key biomaterial: quantum-mechanical simulation of its surfaces in interaction with biomolecules. Physical Chemistry Chemical Physics, 2010, 12, 6309.	1.3	136
57	Thermodynamic Database for Hydrogen Storage Materials. Advances in Science and Technology, 2010, 72, 213-218.	0.2	11
58	Vibrational features of phospho-silicate glasses: Periodic B3LYP simulations. Chemical Physics Letters, 2009, 476, 218-222.	1.2	23
59	H-Bond Features of Fully Hydroxylated Surfaces of Crystalline Silica Polymorphs: A Periodic B3LYP Study. Journal of Physical Chemistry C, 2009, 113, 17876-17884.	1.5	54
60	Water Adsorption on the Stoichiometric (001) and (010) Surfaces of Hydroxyapatite: A Periodic B3LYP Study. Langmuir, 2009, 25, 2188-2198.	1.6	80
61	Ab initio modeling of protein/biomaterial interactions: competitive adsorption between glycine and water onto hydroxyapatite surfaces. Physical Chemistry Chemical Physics, 2009, 11, 9005.	1.3	40
62	Modelling of biomaterials: molecular recognition at the surfaces of bioactive glasses. Acta Crystallographica Section A: Foundations and Advances, 2009, 65, s4-s4.	0.3	0
63	FFSiOH: a New Force Field for Silica Polymorphs and Their Hydroxylated Surfaces Based on Periodic B3LYP Calculations. Chemistry of Materials, 2008, 20, 2522-2531.	3.2	68
64	B3LYP Simulation of the Full Vibrational Spectrum of 45S5 Bioactive Silicate Glass Compared to v-Silica. Chemistry of Materials, 2008, 20, 5610-5621.	3.2	42
65	Ab Initio Modeling of Protein/Biomaterial Interactions: Glycine Adsorption at Hydroxyapatite Surfaces. Journal of the American Chemical Society, 2008, 130, 16181-16183.	6.6	97
66	Periodic B3LYP study of hydroxyapatite (001) surface modelled by thin layer slabs. European Journal of Mineralogy, 2007, 19, 757-767.	0.4	34
67	An ab initio parameterized interatomic force field for hydroxyapatite. Journal of Materials Chemistry, 2007, 17, 2061.	6.7	32
68	A computational multiscale strategy to the study of amorphous materials. Theoretical Chemistry Accounts, 2007, 117, 933-942.	0.5	32
69	Periodic ab initio study of structural and vibrational features of hexagonal hydroxyapatite Ca10(PO4)6(OH)2. Physical Chemistry Chemical Physics, 2006, 8, 2464.	1.3	153
70	In Silico Study of Hydroxyapatite and BioglassÂ®: How Computational Science Sheds Light on Biomaterials. , 0, , .		3
71	Computational Studies of Magnesium and Strontium Substitution in Hydroxyapatite. Key Engineering Materials, 0, 529-530, 123-128.	0.4	3