

# Marta Corno

## List of Publications by Year in descending order

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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	Periodic ab initio study of structural and vibrational features of hexagonal hydroxyapatite $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ . <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 2464.	1.3	153
2	Hydroxyapatite as a key biomaterial: quantum-mechanical simulation of its surfaces in interaction with biomolecules. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6309.	1.3	136
3	<i>Ab Initio</i> Modeling of Protein/Biomaterial Interactions: Glycine Adsorption at Hydroxyapatite Surfaces. <i>Journal of the American Chemical Society</i> , 2008, 130, 16181-16183.	6.6	97
4	Assessment of Different Quantum Mechanical Methods for the Prediction of Structure and Cohesive Energy of Molecular Crystals. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3340-3352.	2.3	85
5	Water Adsorption on the Stoichiometric (001) and (010) Surfaces of Hydroxyapatite: A Periodic B3LYP Study. <i>Langmuir</i> , 2009, 25, 2188-2198.	1.6	80
6	Does Dispersion Dominate over H-Bonds in Drug-Surface Interactions? The Case of Silica-Based Materials As Excipients and Drug-Delivery Agents. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2404-2415.	2.3	72
7	FFSiOH: a New Force Field for Silica Polymorphs and Their Hydroxylated Surfaces Based on Periodic B3LYP Calculations. <i>Chemistry of Materials</i> , 2008, 20, 2522-2531.	3.2	68
8	The vibrational features of hydroxylapatite and type A carbonated apatite: A first principle contribution. <i>American Mineralogist</i> , 2013, 98, 752-759.	0.9	55
9	H-Bond Features of Fully Hydroxylated Surfaces of Crystalline Silica Polymorphs: A Periodic B3LYP Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 17876-17884.	1.5	54
10	Large-Scale B3LYP Simulations of Ibuprofen Adsorbed in MCM-41 Mesoporous Silica as Drug Delivery System. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26737-26749.	1.5	52
11	Coordination chemistry of Ca sites at the surface of nanosized hydroxyapatite: interaction with $\text{H}_2\text{O}$ and CO. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2012, 370, 1313-1336.	1.6	48
12	Silica-Based Materials as Drug Adsorbents: First Principle Investigation on the Role of Water Microsolvation on Ibuprofen Adsorption. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5801-5807.	1.1	47
13	Synthesis and Structural Investigation of $\text{Zr}(\text{BH}_4)_4$ . <i>Journal of Physical Chemistry C</i> , 2012, 116, 20239-20245.	1.5	43
14	B3LYP Simulation of the Full Vibrational Spectrum of 45S5 Bioactive Silicate Glass Compared to v-Silica. <i>Chemistry of Materials</i> , 2008, 20, 5610-5621.	3.2	42
15	Ab initio modeling of protein/biomaterial interactions: competitive adsorption between glycine and water onto hydroxyapatite surfaces. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 9005.	1.3	40
16	Vibrational Properties of $\text{MBH}_4$ and $\text{MBF}_4$ Crystals (M = Li, Na, K): A Combined DFT, Infrared, and Raman Study. <i>Journal of Physical Chemistry C</i> , 2011, 115, 18890-18900.	1.5	39
17	A computational study on the effect of fluorine substitution in $\text{LiBH}_4$ . <i>Journal of Alloys and Compounds</i> , 2011, 509, S679-S683.	2.8	36
18	Stability of the Dipolar (001) Surface of Hydroxyapatite. <i>Journal of Physical Chemistry C</i> , 2012, 116, 6108-6114.	1.5	36

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19	Glycine Adsorption at Nonstoichiometric (010) Hydroxyapatite Surfaces: A B3LYP Study. Journal of Physical Chemistry C, 2012, 116, 14561-14567.	1.5	36
20	Halide Substitution in Magnesium Borohydride. Journal of Physical Chemistry C, 2012, 116, 12482-12488.	1.5	35
21	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
22	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
23	Periodic B3LYP study of hydroxyapatite (001) surface modelled by thin layer slabs. European Journal of Mineralogy, 2007, 19, 757-767.	0.4	34
24	An ab initio parameterized interatomic force field for hydroxyapatite. Journal of Materials Chemistry, 2007, 17, 2061.	6.7	32
25	A computational multiscale strategy to the study of amorphous materials. Theoretical Chemistry Accounts, 2007, 117, 933-942.	0.5	32
26	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
27	Ab initio modelling of protein-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
28	Theoretical and Experimental Study of LiBH <sub>4</sub> -LiCl Solid Solution. Crystals, 2012, 2, 144-158.	1.0	30
29	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
30	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
31	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
32	Vibrational features of phospho-silicate glasses: Periodic B3LYP simulations. Chemical Physics Letters, 2009, 476, 218-222.	1.2	23
33	A thermodynamic investigation of the LiBH <sub>4</sub> -NaBH <sub>4</sub> system. RSC Advances, 2016, 6, 60101-60108.	1.7	23
34	Halide substitution in Ca(BH <sub>4</sub> ) <sub>2</sub> . RSC Advances, 2014, 4, 4736-4742.	1.7	22
35	Elucidating the fundamental forces in protein crystal formation: the case of crambin. Chemical Science, 2016, 7, 1496-1507.	3.7	21
36	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

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37	DFT Modeling of 45S5 and 77S Soda-Lime Phospho-Silicate Glass Surfaces: Clues on Different Bioactivity Mechanism. <i>Langmuir</i> , 2013, 29, 5749-5759.	1.6	20
38	CO <sub>3</sub> <sup>2-</sup> Mobility in Carbonate Apatite As Revealed by Density Functional Modeling. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1364-1369.	1.5	20
39	Phase diagrams of the LiBH <sub>4</sub> -NaBH <sub>4</sub> -KBH <sub>4</sub> system. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25071-25079.	1.3	20
40	Experimental and computational investigations on the AlH <sub>3</sub> /AlF <sub>3</sub> system. <i>Journal of Alloys and Compounds</i> , 2011, 509, 10-14.	2.8	19
41	Revealing Hydroxyapatite Nanoparticle Surface Structure by CO Adsorption: A Combined B3LYP and Infrared Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25526-25534.	1.5	18
42	Properties and Reactivity toward Water of A Type Carbonated Apatite and Hydroxyapatite Surfaces. <i>Journal of Physical Chemistry C</i> , 2018, 122, 3934-3944.	1.5	18
43	Method Dependence of Proline Ring Flexibility in the Poly- <i>l</i> -Proline Type II Polymer. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 370-379.	2.3	16
44	On the Interactions of Melatonin/ $\beta$ -Cyclodextrin Inclusion Complex: A Novel Approach Combining Efficient Semiempirical Extended Tight-Binding (xTB) Results with Ab Initio Methods. <i>Molecules</i> , 2021, 26, 5881.	1.7	16
45	Molecular recognition between membrane epitopes and nearly free surface silanols explains silica membranolytic activity. <i>Colloids and Surfaces B: Biointerfaces</i> , 2022, 217, 112625.	2.5	16
46	How strong are H-bonds at the fully hydroxylated silica surfaces? Insights from the B3LYP electron density topological analysis. <i>Structural Chemistry</i> , 2017, 28, 1009-1015.	1.0	15
47	Probing vibrational modes in silica glass using inelastic neutron scattering with mass contrast. <i>Physical Review B</i> , 2010, 81, .	1.1	14
48	Probing the fate of interstitial water in bulk bioactive glass by ab initio simulations. <i>RSC Advances</i> , 2014, 4, 36425-36436.	1.7	14
49	Solid-State Conformational Flexibility at Work: Energetic Landscape of a Single Crystal-to-Single Crystal Transformation in a Cyclic Hexapeptoid. <i>Crystal Growth and Design</i> , 2021, 21, 897-907.	1.4	13
50	Computational Surface Modelling of Ices and Minerals of Interstellar Interest—Insights and Perspectives. <i>Minerals (Basel, Switzerland)</i> , 2021, 11, 26.	0.8	13
51	Effects of metastability on hydrogen sorption in fluorine substituted hydrides. <i>Journal of Alloys and Compounds</i> , 2014, 615, S706-S710.	2.8	12
52	Theoretical and Experimental Studies of LiBH <sub>4</sub> -LiBr Phase Diagram. <i>ACS Applied Energy Materials</i> , 2021, 4, 7327-7337.	2.5	12
53	Thermodynamic Database for Hydrogen Storage Materials. <i>Advances in Science and Technology</i> , 2010, 72, 213-218.	0.2	11
54	Computational Study of Acidic and Basic Functionalized Crystalline Silica Surfaces as a Model for Biomaterial Interfaces. <i>Langmuir</i> , 2015, 31, 6321-6331.	1.6	11

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55	Models for biomedical interfaces: a computational study of quinone-functionalized amorphous silica surface features. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7793-7806.	1.3	11
56	Solid-State Hydrogen Storage Systems and the Relevance of a Gender Perspective. <i>Energies</i> , 2021, 14, 6158.	1.6	10
57	Balancing Cost and Accuracy in Quantum Mechanical Simulations on Collagen Protein Models. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2566-2574.	2.3	9
58	Simulation of nanosizing effects in the decomposition of Ca(BH <sub>4</sub> ) <sub>2</sub> through atomistic thin film models. <i>Research on Chemical Intermediates</i> , 2021, 47, 345-356.	1.3	7
59	Thermodynamic Tuning of Calcium Hydride by Fluorine Substitution. <i>Materials Research Society Symposia Proceedings</i> , 2012, 1441, 17.	0.1	6
60	Propionic acid derivatives confined in mesoporous silica: monomers or dimers? The case of ibuprofen investigated by static and dynamic ab initio simulations. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	6
61	Ab Initio Modeling of Hydrogen Bond Interaction at Silica Surfaces With Focus on Silica/Drugs Systems. , 2018, , 297-328.		6
62	Ab Initio Computational Study on Fe <sub>2</sub> NiP Schreibersite: Bulk and Surface Characterization. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 1741-1751.	1.2	6
63	In Silico Study of Hydroxyapatite and Bioglass <sup>®</sup> : How Computational Science Sheds Light on Biomaterials. , 0, , .		3
64	Computational Studies of Magnesium and Strontium Substitution in Hydroxyapatite. <i>Key Engineering Materials</i> , 0, 529-530, 123-128.	0.4	3
65	Computing Binding Energies of Interstellar Molecules by Semiempirical Quantum Methods: Comparison Between DFT and GFN2 on Crystalline Ice. <i>Lecture Notes in Computer Science</i> , 2021, , 632-645.	1.0	3
66	Can Mesoporous Silica Speed Up Degradation of Benzodiazepines? Hints from Quantum Mechanical Investigations. <i>Materials</i> , 2022, 15, 1357.	1.3	2
67	Ab initio Calculation of Binding Energies of Interstellar Sulphur-Containing Species on Crystalline Water Ice Models. <i>Lecture Notes in Computer Science</i> , 2021, , 608-619.	1.0	1
68	Water Interaction with Fe <sub>2</sub> NiP Schreibersite (110) Surface: a Quantum Mechanical Atomistic Perspective. <i>Journal of Physical Chemistry C</i> , 2022, 126, 2243-2252.	1.5	1
69	Modelling of biomaterials: molecular recognition at the surfaces of bioactive glasses. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, s4-s4.	0.3	0
70	Surface Modeling of Ceramic Biomaterials. , 2015, , 1-13.		0
71	Surface Modeling of Ceramic Biomaterials. , 2016, , 3935-3947.		0