Antonino Marco Saitta

List of Publications by Year
in descending order

99 papers	6,543 citations	53794 45 h-index	62596 80 g-index
101 all docs	101 docs citations	101 times ranked	7862 citing authors

#	Article	IF	Citations
1	Structure, Stability, Edge States, and Aromaticity of Graphene Ribbons. Physical Review Letters, 2008, 101, 096402.	7.8	582
2	High-pressure Raman spectroscopy study of wurtzite ZnO. Physical Review B, 2002, 65, .	3.2	468
3	Local structure of condensed zinc oxide. Physical Review B, 2003, 68, .	3.2	249
4	Clarâ€™s Theory, Ï€-Electron Distribution, and Geometry of Graphene Nanoribbons. Journal of the American Chemical Society, 2010, 132, 3440-3451.	13.7	219
5	Efficient Approach to Time-Dependent Density-Functional Perturbation Theory for Optical Spectroscopy. Physical Review Letters, 2006, 96, 113001.	7.8	208
6	Influence of a knot on the strength of a polymer strand. Nature, 1999, 399, 46-48.	27.8	206
7	First-principles modeling of the infrared spectrum of kaolinite. American Mineralogist, 2001, 86, 1321-1330.	1.9	201
8	Ab InitioMolecular Dynamics Study of Dissociation of Water under an Electric Field. Physical Review Letters, 2012, 108, 207801.	7.8	181
9	Variations in the work function of doped single- and few-layer graphene assessed by Kelvin probe force microscopy and density functional theory. Physical Review B, 2011, 83, .	3.2	170
10	Ab initiostudy of gap opening and screening effects in gated bilayer graphene. Physical Review B, 2009, 79, .	3.2	147
11	Miller experiments in atomistic computer simulations. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 13768-13773.	7.1	146
12	Van der Waals effects in ab initio water at ambient and supercritical conditions. Journal of Chemical Physics, 2011, 135, 154503.	3.0	138
13	Superconductivity in Dopedsp3Semiconductors: The Case of the Clathrates. Physical Review Letters, 2003, 91, 247001.	7.8	136
14	Doping in Carbon Nanotubes Probed by Raman and Transport Measurements. Physical Review Letters, 2007, 99, 136803.	7.8	135
15	Nature of the Polyamorphic Transition in Ice under Pressure. Physical Review Letters, 2005, 94, 025506.	7.8	120
16	Formation of nucleobases in a Millerâ€“Urey reducing atmosphere. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 4306-4311.	7.1	120
17	Structure and phase diagram of high-density water: The role of interstitial molecules. Physical Review E, 2003, 67, 020201.	2.1	113
18	Formamide reaction network in gas phase and solution via a unified theoretical approach: Toward a reconciliation of different prebiotic scenarios. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 15030-15035.	7.1	111

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19	Sulfur radical species form gold deposits on Earth. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 13484-13489.	7.1	107
20	Kohn anomalies and nonadiabaticity in doped carbon nanotubes. Physical Review B, 2007, 75, .	3.2	103
21	Structure of Dense Liquid Water by Neutron Scattering to 6.5ÂGPa and 670ÂK. Physical Review Letters, 2006, 96, 067801.	7.8	102
22	Unifying description of the wurtzite-to-rocksalt phase transition in wide-gap semiconductors:â€ƒThe effect ofdelectrons on the elastic constants. Physical Review B, 2004, 70, .	3.2	93
23	Structure and stability of graphene nanoribbons in oxygen, carbon dioxide, water, and ammonia. Physical Review B, 2010, 82, .	3.2	85
24	The preparation and structure of salty ice VII under pressure. Nature Materials, 2009, 8, 405-409.	27.5	84
25	First-principles study of OH-stretching modes in kaolinite, dickite, and nacrite. American Mineralogist, 2005, 90, 50-60.	1.9	83
26	Giant Nonadiabatic Effects in Layer Metals: Raman Spectra of Intercalated Graphite Explained. Physical Review Letters, 2008, 100, 226401.	7.8	75
27	Vibrational properties of delafossiteCuGaO2at ambient and high pressures. Physical Review B, 2005, 72, .	3.2	74
28	Structure of the intermediate phase of PbTe at high pressure. Physical Review B, 2005, 71, .	3.2	70
29	Phonon Dispersion of Ice under Pressure. Physical Review Letters, 2004, 93, 225901.	7.8	69
30	First-principles calculation of the infrared spectrum of lizardite. American Mineralogist, 2002, 87, 1286-1290.	1.9	66
31	Translational and Rotational Diffusion in Water in the Gigapascal Range. Physical Review Letters, 2013, 111, 185901.	7.8	66
32	Six-fold-coordinated phosphorus by oxygen in AlPO4 quartz homeotype under high pressure. Nature Materials, 2007, 6, 698-702.	27.5	64
33	High Energy Density Mixed Polymeric Phase from Carbon Monoxide and Nitrogen. Physical Review Letters, 2013, 111, 235501.	7.8	62
34	Effect of salt on the H-bond symmetrization in ice. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 8216-8220.	7.1	58
35	One-step electric-field driven methane and formaldehyde synthesis from liquid methanol. Chemical Science, 2017, 8, 2329-2336.	7.4	56
36	Quantum-driven phase transition in ice described via an efficient Langevin approach. Physical Review B, 2014, 89, .	3.2	55

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37	Structure of Carbon Dioxide Phase IV: Breakdown of the Intermediate Bonding State Scenario. Physical Review Letters, 2009, 103, 185701.	7.8	52
38	Experimental and theoretical evidence for an ionic crystal of ammonia at high pressure. Physical Review B, 2014, 89, .	3.2	52
39	Quantum versus classical protons in pure and salty ice under pressure. Physical Review B, 2016, 93, .	3.2	51
40	Proton Disorder and Superionicity in Hot Dense Ammonia Ice. Physical Review Letters, 2012, 108, 165702.	7.8	50
41	Synthesis of (<scp>d</scp>)-erythrose from glycolaldehyde aqueous solutions under electric field. Chemical Communications, 2018, 54, 3211-3214.	4.1	50
42	Solid ammonia at high pressure: A single-crystal x-ray diffraction study to123GPa. Physical Review B, 2006, 73, .	3.2	49
43	Prebiotic synthesis of nucleic acids and their building blocks at the atomic level â€“ merging models and mechanisms from advanced computations and experiments. Physical Chemistry Chemical Physics, 2016, 18, 20047-20066.	2.8	48
44	Ab initiomolecular-dynamics study of electronic and optical properties of silicon quantum wires: Orientational effects. Physical Review B, 1996, 53, 1446-1451.	3.2	46
45	Polyethylene under tensil load: Strain energy storage and breaking of linear and knotted alkanes probed by first-principles molecular dynamics calculations. Journal of Chemical Physics, 1999, 111, 9434-9440.	3.0	46
46	Structural and Electronic Properties of a Wide-Gap Quaternary Solid Solution: (Zn, Mg) (S, Se). Physical Review Letters, 1998, 80, 4939-4942.	7.8	43
47	Proton Conduction in Water Ices under an Electric Field. Journal of Physical Chemistry B, 2014, 118, 4419-4424.	2.6	41
48	Navigating at Will on the Water Phase Diagram. Physical Review Letters, 2017, 119, 245701.	7.8	41
49	Entropy-based measure of structural order in water. Physical Review E, 2006, 73, 040502.	2.1	40
50	Strong electric fields at a prototypical oxide/water interface probed by ab initio molecular dynamics: MgO(001). Physical Chemistry Chemical Physics, 2015, 17, 20382-20390.	2.8	39
51	Probing the electrostatic environment of bilayer graphene using Raman spectra. Physical Review B, 2009, 80, .	3.2	38
52	Hydrothermal Decomposition of Amino Acids and Origins of Prebiotic Meteoritic Organic Compounds. ACS Earth and Space Chemistry, 2018, 2, 588-598.	2.7	37
53	Ab initio molecular dynamics study of an aqueous NaCl solution under an electric field. Physical Chemistry Chemical Physics, 2016, 18, 23164-23173.	2.8	36
54	Multiple Ionic-Plasmon Resonances in Naturally Occurring Multiwall Nanotubes: Infrared Spectra of Chrysotile Asbestos. Physical Review Letters, 2002, 89, 177401.	7.8	34

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55	Statistical entropy and density maximum anomaly in liquid water. Journal of Chemical Physics, 2003, 119, 3587-3589.	3.0	34
56	High density amorphous ices: Disordered water towards close packing. Journal of Chemical Physics, 2004, 121, 8430.	3.0	34
57	Pressure-Induced Polyamorphism in Salty Water. Physical Review Letters, 2011, 106, 125701.	7.8	33
58	Liquid methanol under a static electric field. Journal of Chemical Physics, 2015, 142, 054502.	3.0	32
59	In situneutron diffraction studies of high density amorphous ice under pressure. Journal of Physics Condensed Matter, 2005, 17, S967-S974.	1.8	31
60	Raman spectrum of ammonia IV. Physical Review B, 2006, 74, .	3.2	31
61	Novel superconducting skutterudite-type phosphorus nitride at high pressure from first-principles calculations. Scientific Reports, 2014, 4, 5889.	3.3	29
62	Generating Converged Accurate Free Energy Surfaces for Chemical Reactions with a Force-Matched Semiempirical Model. Journal of Chemical Theory and Computation, 2018, 14, 2207-2218.	5.3	28
63	First-Principles Molecular Dynamics Study of the Rupture Processes of a Bulklike Polyethylene Knot. Journal of Physical Chemistry B, 2001, 105, 6495-6499.	2.6	26
64	First-Principles Study of Bond Rupture of Entangled Polymer Chains. Journal of Physical Chemistry B, 2000, 104, 2197-2200.	2.6	25
65	Prebiotic chemistry and origins of life research with atomistic computer simulations. Physics of Life Reviews, 2020, 34-35, 105-135.	2.8	25
66	Fully Quantum Description of the Zundel Ion: Combining Variational Quantum Monte Carlo with Path Integral Langevin Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 2400-2417.	5.3	24
67	Entropy from Correlations in TIP4P Water. Journal of Chemical Theory and Computation, 2010, 6, 625-636.	5.3	22
68	Novel electrochemical route to cleaner fuel dimethyl ether. Scientific Reports, 2017, 7, 6901.	3.3	22
69	Synthesis of RNA Nucleotides in Plausible Prebiotic Conditions from ab Initio Computer Simulations. Journal of Physical Chemistry Letters, 2018, 9, 4981-4987.	4.6	22
70	Effect of Electric Field Orientation on the Mechanical and Electrical Properties of Water Ices: An Ab-initio Study. Journal of Physical Chemistry B, 2014, 118, 12717-12724.	2.6	21
71	Evolution of Fragments Formed at the Rupture of a Knotted Alkane Molecule. Journal of the American Chemical Society, 1999, 121, 11827-11830.	13.7	20
72	Probing ice VII crystallization from amorphous NaClâ€“D₂O solutions at gigapascal pressures. Physical Chemistry Chemical Physics, 2017, 19, 1875-1883.	2.8	19

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73	Proton tunneling in fatty acid/soap crystals?. Journal of Chemical Physics, 2003, 118, 1-3.	3.0	18
74	Quantum Monte Carlo Study of the Protonated Water Dimer. Journal of Chemical Theory and Computation, 2014, 10, 1980-1993.	5.3	18
75	Stability of 2â€²,3â€² and 3â€²,5â€² cyclic nucleotides in formamide and in water: a theoretical insight into the factors controlling the accumulation of nucleic acid building blocks in a prebiotic pool. Physical Chemistry Chemical Physics, 2017, 19, 1817-1825.	2.8	18
76	Structural characterization of eutectic aqueous NaCl solutions under variable temperature and pressure conditions. Physical Chemistry Chemical Physics, 2015, 17, 14054-14063.	2.8	17
77	Step by Step Strecker Amino Acid Synthesis from Ab Initio Prebiotic Chemistry. Journal of Physical Chemistry Letters, 2021, 12, 2630-2637.	4.6	17
78	Ab Initio Molecular Dynamics Study of Methanol-Water Mixtures under External Electric Fields. Molecules, 2020, 25, 3371.	3.8	15
79	Effects of disorder on the optical gap of (Zn,Mg)(S,Se). Applied Physics Letters, 1999, 75, 2746-2748.	3.3	14
80	The trisulfur radical ion S ₃ ^{â€¢â˜} controls platinum transport by hydrothermal fluids. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	13
81	Phonon Softening and Elastic Instabilities in the Cubic-to-Orthorhombic Structural Transition of CsH. Physical Review Letters, 1997, 78, 4958-4961.	7.8	11
82	Formic Acid Synthesis in a Waterâ€“Mineral System: Major Role of the Interface. Journal of Physical Chemistry C, 2020, 124, 5125-5131.	3.1	11
83	Influence of a knot on the stretching-induced crystallization of a polymer. Journal of Chemical Physics, 2002, 116, 5333-5336.	3.0	9
84	Structural Properties of the Amorphous Ices:Â An Analysis in Terms of Distance-Ranked Neighbors and Angular Correlationsâ€. Journal of Physical Chemistry B, 2006, 110, 3595-3603.	2.6	9
85	The thermodynamic stability and simulated STM images of graphene nanoribbons. Physica Status Solidi (B): Basic Research, 2009, 246, 2586-2591.	1.5	9
86	On the link between polyamorphism and liquid-liquid transition: The case of salty water. Journal of Chemical Physics, 2019, 151, 044503.	3.0	9
87	Rubidium localization in single-walled carbon nanotube bundles: Structural study. Physical Review B, 2008, 78, .	3.2	8
88	Gold speciation in hydrothermal fluids revealed by in situ high energy resolution X-ray absorption spectroscopy. American Mineralogist, 2022, 107, 369-376.	1.9	8
89	KlotzetÂal.Reply:. Physical Review Letters, 2006, 96, .	7.8	7
90	Disorder-order phase transition at high pressure in ammonium fluoride. Physical Review B, 2017, 96, .	3.2	7

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91	First-principles study of an iron-based molecule grafted on graphene. Europhysics Letters, 2011, 96, 57001.	2.0	6
92	Reply to Bada and Cleaves: Ab initio free-energy landscape of Miller-like prebiotic reactions. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E343-4.	7.1	6
93	Polymeric phase V of carbon dioxide has not been recovered at ambient pressure and has a unique structure. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E656-E657.	7.1	5
94	Pressure Dependence of Wurtzite ZnO Structure. High Pressure Research, 2002, 22, 365-367.	1.2	4
95	Free Energy Calculations of Electric Field-Induced Chemistry. Challenges and Advances in Computational Chemistry and Physics, 2019, , 95-126.	0.6	3
96	Chemical Decomposition of the TFSI Anion under Aqueous Basic Conditions. , 2022, 1, .		3
97	Temperature-induced topological differentiation of the two high-density amorphous ices. Europhysics Letters, 2006, 74, 445-451.	2.0	2
98	Breakdown of the adiabatic approximation in a doped graphene monolayer and in metallic carbon nanotubes. Physica Status Solidi (B): Basic Research, 2007, 244, 4118-4123.	1.5	2
99	Reply to comments on â€œPrebiotic chemistry and origins of life research with atomistic computer simulationsâ€• Physics of Life Reviews, 2020, 34-35, 153-155.	2.8	0