Simone Taioli

List of Publications by Year
in descending order

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68	2,203	218677	223800
papers	citations	26 h-index	46 g-index

71	71	71	3292
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Production and processing of graphene and related materials. 2D Materials, 2020, 7, 022001.	4.4	333
2	Tunable Band Gap in Hydrogenated Quasi-Free-Standing Graphene. Nano Letters, 2010, 10, 3360-3366.	9.1	297
3	Zeolitic imidazolate frameworks for separation of binary mixtures of CO2, CH4, N2 and H2: A computer simulation investigation. Microporous and Mesoporous Materials, 2011, 143, 46-53.	4.4	136
4	Melting curve of tantalum from first principles. Physical Review B, 2007, 75, .	3.2	99
5	UV-Light-Induced Vibrational Coherences: The Key to Understand Kasha Rule Violation in trans-Azobenzene. Journal of Physical Chemistry Letters, 2018, 9, 1534-1541.	4.6	96
6	Ab initiomelting curve of molybdenum by the phase coexistence method. Journal of Chemical Physics, 2007, 126, 194502.	3.0	89
7	A Quantum Chemical Interpretation of Two-Dimensional Electronic Spectroscopy of Light-Harvesting Complexes. Journal of the American Chemical Society, 2017, 139, 7558-7567.	13.7	71
8	Spider silk reinforced by graphene or carbon nanotubes. 2D Materials, 2017, 4, 031013.	4.4	57
9	Electron spectroscopies and inelastic processes in nanoclusters and solids: Theory and experiment. Physics Reports, 2010, 493, 237-319.	25.6	55
10	Direct observation of a dispersionless impurity band in hydrogenated graphene. Physical Review B, 2011, 83, .	3.2	49
11	Infrared spectroscopy of copper-resveratrol complexes: A joint experimental and theoretical study. Journal of Chemical Physics, 2012, 137, 024307.	3.0	46
12	Communication: Electronic band gaps of semiconducting zig-zag carbon nanotubes from many-body perturbation theory calculations. Journal of Chemical Physics, 2012, 136, 181101.	3.0	43
13	Designing graphene based nanofoams with nonlinear auxetic and anisotropic mechanical properties under tension or compression. Carbon, 2017, 111, 796-806.	10.3	39
14	Mechanical and thermal properties of graphene random nanofoams via Molecular Dynamics simulations. Carbon, 2018, 132, 766-775.	10.3	39
15	Mixedab initioquantum mechanical and Monte Carlo calculations of secondary emission fromSiO2nanoclusters. Physical Review B, 2009, 79, .	3.2	37
16	On the angular dependence of L x-ray production cross sections following photoionization at an energy of 59.54 keV. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, 843-851.	1.5	34
17	SURPRISES: when ab initio meets statistics in extended systems. Computational Science & Discovery, 2009, 2, 015002.	1.5	33
18	2D Material Armors Showing Superior Impact Strength of Few Layers. ACS Applied Materials & Interfaces, 2017, 9, 40820-40830.	8.0	32

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19	Modeling flexibility in metalâ€“organic frameworks: Comparison between Density-Functional Tight-Binding and Universal Force Field approaches for bonded interactions. Microporous and Mesoporous Materials, 2012, 163, 215-220.	4.4	31
20	Synthesis of single layer graphene on Cu(111) by C₆₀ supersonic molecular beam epitaxy. RSC Advances, 2016, 6, 37982-37993.	3.6	31
21	Gas adsorption and dynamics in Pillared Graphene Frameworks. Microporous and Mesoporous Materials, 2018, 257, 222-231.	4.4	31
22	Epitaxy of Nanocrystalline Silicon Carbide on Si(111) at Room Temperature. Journal of the American Chemical Society, 2012, 134, 17400-17403.	13.7	30
23	Gas Adsorption and Separation in Realistic and Idealized Frameworks of Organic Pillared Graphene: A Comparative Study. Journal of Physical Chemistry C, 2015, 119, 1980-1987.	3.1	29
24	THEORETICAL ESTIMATES OF STELLARe^{â€“}CAPTURES. I. THE HALF-LIFE OF⁷Be IN EVOLVED STARS. Astrophysical Journal, 2013, 764, 118.	4.5	27
25	Computational study of graphene growth on copper by first-principles and kinetic Monte Carlo calculations. Journal of Molecular Modeling, 2014, 20, 2260.	1.8	27
26	Electronic properties of extended graphene nanomaterials from GW calculations. Physica Status Solidi (B): Basic Research, 2009, 246, 2572-2576.	1.5	26
27	Multiscale Investigation of Oxygen Vacancies in TiO₂ Anatase and Their Role in Memristorâ€™s Behavior. Journal of Physical Chemistry C, 2016, 120, 22045-22053.	3.1	24
28	Presolar Grain Isotopic Ratios as Constraints to Nuclear and Stellar Parameters of Asymptotic Giant Branch Star Nucleosynthesis. Astrophysical Journal, 2021, 921, 7.	4.5	23
29	Secondary electron emission and yield spectra of metals from Monte Carlo simulations and experiments. Journal of Physics Condensed Matter, 2019, 31, 055901.	1.8	22
30	Monte Carlo simulations of measured electron energy-loss spectra of diamond and graphite: Role of dielectric-response models. Carbon, 2017, 118, 299-309.	10.3	21
31	Lobachevsky crystallography made real through carbon pseudospheres. Journal of Physics Condensed Matter, 2016, 28, 13LT01.	1.8	20
32	A Novel Approach to Î²-Decay: PANDORA, a New Experimental Setup for Future In-Plasma Measurements. Universe, 2022, 8, 80.	2.5	19
33	Electron-molecule collisions at low and intermediate energies using the R-matrix method. European Physical Journal D, 2005, 35, 231-237.	1.3	18
34	Structural, electronic and mechanical properties of all-sp2 carbon allotropes with density lower than graphene. Carbon, 2020, 159, 512-526.	10.3	18
35	Relative Role of Physical Mechanisms on Complex Biodamage Induced by Carbon Irradiation. Journal of Physical Chemistry Letters, 2021, 12, 487-493.	4.6	15
36	Anisotropic Approach for Simulating Electron Transport in Layered Materials: Computational and Experimental Study of Highly Oriented Pyrolitic Graphite. Journal of Physical Chemistry C, 2018, 122, 10159-10166.	3.1	14

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37	Effects of a revised ⁷Be e^{â”}-capture rate on solar neutrino fluxes. Astronomy and Astrophysics, 2019, 623, A126.	5.1	13
38	Exploring event horizons and Hawking radiation through deformed graphene membranes. 2D Materials, 2020, 7, 041006.	4.4	13
39	A wave packet method for treating nuclear dynamics on complex potentials. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, 4379-4392.	1.5	12
40	Non-adiabatic ab initio molecular dynamics of supersonic beam epitaxy of silicon carbide at room temperature. Journal of Chemical Physics, 2013, 138, 044701.	3.0	12
41	Melting curve and Hugoniot of molybdenum up to 400 GPa byab initiosimulations. Journal of Physics: Conference Series, 2008, 121, 012009.	0.4	11
42	Electronic excitation spectra of cerium oxides: from ab initio dielectric response functions to Monte Carlo electron transport simulations. Physical Chemistry Chemical Physics, 2021, 23, 19173-19187.	2.8	10
43	Theoretical Estimate of the Half-life for the Radioactive ¹³⁴Cs and ¹³⁵Cs in Astrophysical Scenarios. Astrophysical Journal, 2022, 933, 158.	4.5	10
44	Finite-range effects in dilute Fermi gases at unitarity. Physical Review A, 2011, 84, .	2.5	8
45	A Computational Perspective on Multichannel Scattering Theory with Applications to Physical and Nuclear Chemistry. Annual Reports in Computational Chemistry, 2015, 11, 191-310.	1.7	8
46	Nuclear Beta Decay: Relativistic Theory and Ab Initio Simulations of Electroweak Decay Spectra in Mediumâ€Heavy Nuclei and of Atomic and Molecular Electronic Structure (Adv. Theory Simul. 11/2018). Advanced Theory and Simulations, 2018, 1, 1870030.	2.8	8
47	A comparison between Monte Carlo method and the numerical solution of the Ambartsumian-Chandrasekhar equations to unravel the dielectric response of metals. Computational Materials Science, 2020, 173, 109420.	3.0	8
48	Ab initiocalculation of the normal Auger spectrum of C2H2. Journal of Physics B: Atomic, Molecular and Optical Physics, 2004, 37, 1237-1244.	1.5	7
49	Ab initio calculation of the C1s photoelectron spectrum of C2H2. Nuclear Instruments & Methods in Physics Research B, 2004, 213, 65-70.	1.4	7
50	Energy Deposition around Swift Carbon-Ion Tracks in Liquid Water. International Journal of Molecular Sciences, 2022, 23, 6121.	4.1	7
51	Auger-electron angular distributions calculated without the two-step approximation: Calculation of angle-resolved resonant Auger spectra ofC2H2. Physical Review A, 2004, 70, .	2.5	6
52	WATERWAVES: wave particles dynamics on a complex triatomic potential. Computer Physics Communications, 2006, 175, 41-51.	7.5	6
53	Understanding anharmonic effects on hydrogen desorption characteristics of Mg_nH_{2n} nanoclusters by ab initio trained deep neural network. Nanoscale, 2022, 14, 5589-5599.	5.6	6
54	The Interaction of C60 on Si(111) 7Ã¢â‚¬Ãƒâ€”Ã¢â‚¬7 Studied by Supersonic Molecular Beams: Interplay between Precursor Kinetic Energy and Substrate Temperature in Surface Activated Processes. Frontiers in Materials, 2015, 2, .	2.4	5

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55	A novel combined experimental and multiscale theoretical approach to unravel the structure of SiC/SiO_x core/shell nanowires for their optimal design. Nanoscale, 2018, 10, 13449-13461.	5.6	5
56	Ab-initio melting curve and principal Hugoniot of tantalum. Journal of Physics: Conference Series, 2008, 121, 012010.	0.4	4
57	Tetrapeptide unfolding dynamics followed by core-level spectroscopy: a first-principles approach. Physical Chemistry Chemical Physics, 2015, 17, 11269-11276.	2.8	4
58	The Resonant and Normal Auger Spectra of Ozone. Symmetry, 2021, 13, 516.	2.2	4
59	Computational methods for 2D materials modelling. Reports on Progress in Physics, 2021, 84, 106501.	20.1	4
60	Lithium abundances in AGB stars and a new estimate for the⁷Be life-time. Journal of Physics: Conference Series, 2016, 665, 012014.	0.4	2
61	Ultrafast Carotenoid to Retinal Energy Transfer in Xanthorhodopsin Revealed by the Combination of Transient Absorption and Twoâ€Dimensional Electronic Spectroscopy. Chemistry - A European Journal, 2018, 24, 12084-12092.	3.3	2
62	Relativistic Theory and Ab Initio Simulations of Electroweak Decay Spectra in Mediumâ€Heavy Nuclei and of Atomic and Molecular Electronic Structure. Advanced Theory and Simulations, 2018, 1, 1800086.	2.8	2
63	Relativistic quantum theory and algorithms: A toolbox for modeling many-fermion systems in different scenarios. Annual Reports in Computational Chemistry, 2021, 17, 55-111.	1.7	2
64	A scattering view of the Bogoliubov-de Gennes equations. , 2012, , .		1
65	The BEC-BCS crossover in ultracold Fermi gases beyond the contact-potential approximation. European Physical Journal D, 2013, 67, 1.	1.3	1
66	Editorial: New Frontiers in Multiscale Modelling of Advanced Materials. Frontiers in Materials, 2015, 2, .	2.4	1
67	Enabling Materials By Dimensionality: From 0D to 3D Carbon-Based Nanostructures. , 2020, , 135-200.		1
68	A Birdâ€™s Eye View on the Concept of Multichannel Scattering with Applications to Materials Science, Condensed Matter, and Nuclear Astrophysics. Frontiers in Materials, 2015, 2, .	2.4	0