Fausto Cargnoni

List of Publications by Year
in descending order

50 papers	19,490 citations	393982 19 h-index	205818 48 g-index
53 all docs	53 docs citations	53 times ranked	22564 citing authors

#	Article	IF	Citations
1	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	0.7	18,183
2	Interstitial Zn Atoms Do the Trick in Thermoelectric Zinc Antimonide, Zn4Sb3: A Combined Maximum Entropy Method X-ray Electron Density and Ab Initio Electronic Structure Study. Chemistry - A European Journal, 2004, 10, 3861-3870.	1.7	169
3	Chemical information from the source function. Journal of Computational Chemistry, 2003, 24, 422-436.	1.5	160
4	Nearâ€IR Emitting Iridium(III) Complexes with Heteroaromatic Î²â€Diketonate Ancillary Ligands for Efficient Solutionâ€Processed OLEDs: Structureâ€“Property Correlations. Angewandte Chemie - International Edition, 2016, 55, 2714-2718.	7.2	126
5	Fundamental Properties and Nature of CHÂ·Â·O Interactions in Crystals on the Basis of Experimental and Theoretical Charge Densities. The Case of 3,4-Bis(dimethylamino)-3-cyclobutene-1,2-dione (DMACB) Crystal. Journal of Physical Chemistry A, 2002, 106, 2707-2720.	1.1	118
6	Formation and annihilation of a bond defect in silicon: Anab initioquantum-mechanical characterization. Physical Review B, 1998, 57, 170-177.	1.1	73
7	Chemical insight into electron density and wave functions: software developments and applications to crystals, molecular complexes and materials science. Theoretical Chemistry Accounts, 2007, 117, 847-884.	0.5	48
8	An experimental (120â€…K) and theoretical electron-density study of KMnO4and KClO4. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 494-501.	0.3	47
9	Evolution of energetics and bonding of compact self-interstitial clusters in Si. Europhysics Letters, 2000, 50, 608-614.	0.7	45
10	Predicting atomic dopant solvation in helium clusters: The MgHen case. Journal of Chemical Physics, 2005, 123, 054328.	1.2	38
11	Picosecond solvation dynamics of alkali cations in superfluid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mmultiscripts><mml:mi mathvariant="normal">He</mml:mi><mml:mprescripts /><mml:none /><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:mmultiscripts></mml:math>nanodroplets. Physical Review B, 2014, 90, .	1.1	33
12	An ab initio investigation of the Heâ€“H2O complex. Chemical Physics Letters, 2003, 370, 233-239.	1.2	32
13	Ground state potential energy surfaces and bound states of Mâ€“He dimers (M=Cu,Ag,Au): A theoretical investigation. Journal of Chemical Physics, 2008, 129, 204307.	1.2	30
14	Communication: Nucleation of quantized vortex rings in 4He nanodroplets. Journal of Chemical Physics, 2014, 140, 131101.	1.2	29
15	Unraveling the Degradation Mechanism in FIrpic-Based Blue OLEDs: II. Trap and Detect Molecules at the Interfaces. Chemistry of Materials, 2019, 31, 2277-2285.	3.2	27
16	Germanium K edge in GeO2 polymorphs. Correlation between local coordination and electronic structure of germanium. Physical Chemistry Chemical Physics, 2003, 5, 1451-1456.	1.3	24
17	A cascade mechanism for a simple reaction: The gas-phase methylation of phenol with methanol. Journal of Catalysis, 2019, 370, 447-460.	3.1	23
18	The electronic structure of nitrilimine: absence of the carbenic form. Chemical Communications, 2006, , 1030.	2.2	22

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19	Unveiling the acetone sensing mechanism by <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msub><mml:mrow><mml:mi mathvariant="normal">WO</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math> chemiresistors through a joint theory-experiment approach. Electrochimica Acta, 2021, 371, 137611.	2.6	21
20	Solubility of Metal Atoms in Helium Droplets: Exploring the Effect of the Well Depth Using the Coinage Metals Cu and Ag. Journal of Physical Chemistry A, 2011, 115, 7141-7152.	1.1	20
21	Potential energy surface, bound states, and rotational inelastic cross sections of the He-CH[sub 4] system: A theoretical investigation. Journal of Chemical Physics, 2004, 121, 8261.	1.2	17
22	Upper limit to the ultimate achievable emission wavelength in near-IR emitting cyclometalated iridium complexes. Photochemical and Photobiological Sciences, 2017, 16, 1220-1223.	1.6	17
23	Hydrogen diffusion in crystalline SiO2. Chemical Physics Letters, 1997, 264, 435-440.	1.2	16
24	Geometrical reconstructions and electronic relaxations of silicon surfaces. I. An electron density topological study of H-covered and clean Si(111)(1Ã—1) surfaces. Journal of Chemical Physics, 2000, 112, 887-899.	1.2	16
25	Spin asymmetric band gap opening in graphene by Fe adsorption. Surface Science, 2015, 634, 62-67.	0.8	16
26	Dynamics of photoexcited Ba+ cations in 4He nanodroplets. Journal of Chemical Physics, 2016, 144, 094302.	1.2	15
27	An MOâˆ’VB Approach for the Determination of Intermolecular Forces. Theory and Calculations on the He2, Heâˆ’CH4, and Heâˆ’H2O Systems. Journal of Physical Chemistry A, 2002, 106, 5521-5528.	1.1	12
28	Exciplexes with Ionic Dopants: Stability, Structure, and Experimental Relevance of M+(2P)4Hen (M = Sr,) Tj ETQq0 0 0 rgBT /Overlock 10	1.1	10
29	Direct-space analysis of the Si-Si bonding pattern in the Ï€-bonded chain reconstructed Si(111)(2 Ã— 1) surface. Theoretical Chemistry Accounts, 2001, 105, 309-322.	0.5	9
30	A Theoretical Study on the Rotational Motion and Interactions in the Disordered Phase of MBH₄ (M = Li, Na, K, Rb, Cs). Journal of Physical Chemistry C, 2013, 117, 2308-2316.	1.5	9
31	Coinage metal exciplexes with helium atoms: a theoretical study of M*(2L)Hen (M = Cu, Ag, Au; L = P,D). Physical Chemistry Chemical Physics, 2013, 15, 18410.	1.3	9
32	Unraveling the Degradation Mechanism of FIrpic-Based Blue OLEDs: I. A Theoretical Investigation. Chemistry of Materials, 2019, 31, 2269-2276.	3.2	9
33	Mapping the complete bonding network in KBH4 using the combined power of powder diffraction and maximum entropy method. Computational and Theoretical Chemistry, 2015, 1053, 245-253.	1.1	7
34	Spin-polarized charge transfer induced by transition metal adsorption on graphene. Physica Scripta, 2016, 91, 053007.	1.2	7
35	Understanding the Reorientational Dynamics of Solid-State MBH₄ (M = Liâ€“Cs). Journal of Physical Chemistry C, 2015, 119, 12109-12118.	1.5	6
36	Î²-Diketonate ancillary ligands in heteroleptic iridium complexes: a balance between synthetic advantages and photophysical troubles. Photochemical and Photobiological Sciences, 2018, 17, 1169-1178.	1.6	6

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37	Experimental and theoretical insight into the mechanism of CO2 cycloaddition to epoxides catalyzed by ammonium ferrates. Journal of CO2 Utilization, 2022, 62, 102062.	3.3	6
38	Spin-filtering in graphene junctions with Ti and Co adsorbates. Chemical Physics, 2016, 478, 91-96.	0.9	5
39	Ab Initio Many-Body Perturbation Theory Calculations of the Electronic and Optical Properties of Cyclometalated Ir(III) Complexes. Journal of Chemical Theory and Computation, 2020, 16, 1188-1199.	2.3	5
40	Direct-space analysis of the electronic structure of the YBa2Cu3O6 and YBa2Cu3O7 crystals. Canadian Journal of Chemistry, 2002, 80, 235-244.	0.6	4
41	Application of valence-bond techniques to the study of weakly bound complexes. The potential energy surface of the Neâ€“CH4system. Physical Chemistry Chemical Physics, 2007, 9, 2457-2469.	1.3	4
42	Helium-induced electronic transitions in photo-excited Ba+â€“Hen exciplexes. Journal of Chemical Physics, 2018, 148, 144302.	1.2	4
43	Magnetic Moments and Electron Transport through Chromium-Based Antiferromagnetic Nanojunctions. Materials, 2018, 11, 2030.	1.3	3
44	The azideâ€“alkyne cycloaddition catalysed by transition metal oxide nanoparticles. New Journal of Chemistry, 2019, 43, 18049-18061.	1.4	3
45	A theoretical investigation on the chemical bonding of interstitial and vacancy defects in silicon during their migration. Nuclear Instruments & Methods in Physics Research B, 1997, 127-128, 235-238.	0.6	2
46	Structure, energetics, clustering and migration of point-defects in silicon. Physica Scripta, 1996, T66, 207-211.	1.2	2
47	Electronic Structure and Magnetic Coupling of Pure and Mg-Doped KCuF3. Advances in Condensed Matter Physics, 2018, 2018, 1-10.	0.4	1
48	Organic Spintronics: A Theoretical Investigation of a Graphene-Porphyrin Based Nanodevice. Magnetochemistry, 2020, 6, 27.	1.0	1
49	A Chemical Approacht o the First-Principles Modeling of Novel Thermoelectric Materials. , 2005, , 7-1-7-13.		1
50	Results and perspectives of the MOâ€“VB method. Application examples on the He2 and the LiHâ€“He complexes. Physical Chemistry Chemical Physics, 2010, 12, 4224.	1.3	0