Fausto Cargnoni

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6318294/publications.pdf

Version: 2024-02-01

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	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
2	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
3	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
4	Organic Spintronics: A Theoretical Investigation of a Graphene-Porphyrin Based Nanodevice. Magnetochemistry, 2020, 6, 27.	1.0	1
5	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
6	Unraveling the Degradation Mechanism of FIrpic-Based Blue OLEDs: I. A Theoretical Investigation. Chemistry of Materials, 2019, 31, 2269-2276.	3.2	9
7	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
8	The azideâ€“alkyne cycloaddition catalysed by transition metal oxide nanoparticles. New Journal of Chemistry, 2019, 43, 18049-18061.	1.4	3
9	Helium-induced electronic transitions in photo-excited Ba+â€“Hen exciplexes. Journal of Chemical Physics, 2018, 148, 144302.	1.2	4
10	Electronic Structure and Magnetic Coupling of Pure and Mg-Doped KCuF3. Advances in Condensed Matter Physics, 2018, 2018, 1-10.	0.4	1
11	Magnetic Moments and Electron Transport through Chromium-Based Antiferromagnetic Nanojunctions. Materials, 2018, 11, 2030.	1.3	3
12	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
13	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
14	Dynamics of photoexcited Ba+ cations in 4He nanodroplets. Journal of Chemical Physics, 2016, 144, 094302.	1.2	15
15	Spin-polarized charge transfer induced by transition metal adsorption on graphene. Physica Scripta, 2016, 91, 053007.	1.2	7
16	Spin-filtering in graphene junctions with Ti and Co adsorbates. Chemical Physics, 2016, 478, 91-96.	0.9	5
17	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
18	Understanding the Reorientational Dynamics of Solid-State MBH₄ (M = Liâ€“Cs). Journal of Physical Chemistry C, 2015, 119, 12109-12118.	1.5	6

#	Article	IF	Citations
19	Spin asymmetric band gap opening in graphene by Fe adsorption. Surface Science, 2015, 634, 62-67.	0.8	16
20	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
21	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
22	Communication: Nucleation of quantized vortex rings in 4He nanodroplets. Journal of Chemical Physics, 2014, 140, 131101.	1.2	29
23	Exciplexes with Ionic Dopants: Stability, Structure, and Experimental Relevance of M+(2P)4Hen (M = Sr,) Tj ETQq1 1 0.784314 rgBT /Ov	1.1	10
24	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
25	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
26	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
27	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
28	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
29	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
30	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
31	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
32	The electronic structure of nitrilimine: absence of the carbenic form. Chemical Communications, 2006, , 1030.	2.2	22
33	Predicting atomic dopant solvation in helium clusters: The MgHen case. Journal of Chemical Physics, 2005, 123, 054328.	1.2	38
34	A Chemical Approacht o the First-Principles Modeling of Novel Thermoelectric Materials. , 2005, , 7-1-7-13.		1
35	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
36	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

#	Article	IF	Citations
37	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
38	Chemical information from the source function. Journal of Computational Chemistry, 2003, 24, 422-436.	1.5	160
39	An ab initio investigation of the Heâ€“H2O complex. Chemical Physics Letters, 2003, 370, 233-239.	1.2	32
40	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
41	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
42	Direct-space analysis of the electronic structure of the YBa2Cu3O6 and YBa2Cu3O7 crystals. Canadian Journal of Chemistry, 2002, 80, 235-244.	0.6	4
43	An MOâ^'VB Approach for the Determination of Intermolecular Forces. Theory and Calculations on the He2, Heâ^'CH4, and Heâ^'H2O Systems. Journal of Physical Chemistry A, 2002, 106, 5521-5528.	1.1	12
44	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
45	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
46	Evolution of energetics and bonding of compact self-interstitial clusters in Si. Europhysics Letters, 2000, 50, 608-614.	0.7	45
47	Formation and annihilation of a bond defect in silicon: Anab initioquantum-mechanical characterization. Physical Review B, 1998, 57, 170-177.	1.1	73
48	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
49	Hydrogen diffusion in crystalline SiO2. Chemical Physics Letters, 1997, 264, 435-440.	1.2	16
50	Structure, energetics, clustering and migration of point-defects in silicon. Physica Scripta, 1996, T66, 207-211.	1.2	2