Davide Ceresoli

List of Publications by Year
in descending order

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84	25,431	159585	60623
papers	citations	30 h-index	81 g-index

85	85	85	24986
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advancing Near-Infrared Phosphorescence with Heteroleptic Iridium Complexes Bearing a Single Emitting Ligand: Properties and Organic Light-Emitting Diode Applications. Chemistry of Materials, 2022, 34, 574-583.	6.7	20
2	Anharmonic motion and aspherical nuclear probability density functions in cesium halides. Physical Review B, 2022, 105, .	3.2	0
3	GIPAW Pseudopotentials of d Elements for Solid-State NMR. Materials, 2022, 15, 3347.	2.9	4
4	High pressure structure studies of three SrGeO3 polymorphs â€“ Amorphization under pressure. Journal of Alloys and Compounds, 2021, 855, 157419.	5.5	3
5	Firstâ€Principles Study on the Crystalline Ga 4 Sb 6 Te 3 Phase Change Compound. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2000382.	2.4	2
6	Comparative Analysis of DFT+U, ACBN0, and Hybrid Functionals on the Spin Density of YTiO3 and SrRuO3. Applied Sciences (Switzerland), 2021, 11, 616.	2.5	1
7	Electronic structure of defected polyethylene for Schottky emission. Materials Chemistry and Physics, 2021, 263, 124268.	4.0	6
8	First-Principles Study on Electron-Induced Excitations of Atomic Layer Deposition Precursors: Inelastic Electron Wave Packet Scattering with Cobalt Tricarbonyl Nitrosyl Co(CO)3NO Using Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2021, 125, 4524-4533.	2.5	2
9	About the deterioration of polyethylene exposed to plasma discharges: A comparison between two models. Applied Surface Science, 2021, 567, 150306.	6.1	3
10	Advanced modeling of materials with PAOFLOW 2.0: New features and software design. Computational Materials Science, 2021, 200, 110828.	3.0	21
11	eQE 2.0: Subsystem DFT beyond GGA functionals. Computer Physics Communications, 2021, 269, 108122.	7.5	13
12	High-Pressure Computational Search of Trivalent Lanthanide Dinitrides. Journal of Physical Chemistry C, 2021, 125, 161-167.	3.1	5
13	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.	5.3	5
14	High-pressure, low-temperature studies of phase transitions in SrRuO3 â€“ Absence of volume collapse. Journal of Solid State Chemistry, 2020, 287, 121360.	2.9	2
15	Local Structure and Magnetism of Fe2O3 Maghemite Nanocrystals: The Role of Crystal Dimension. Nanomaterials, 2020, 10, 867.	4.1	37
16	First-principles evaluation of the secondary electron yield (Î³^N) from polyethylene surface. Journal Physics D: Applied Physics, 2020, 53, 175301.	2.8	6
17	Investigation of the high pressure phase BiS2: Temperature-resolved structure and compression behavior to 60â€¯GPa. Journal of Alloys and Compounds, 2019, 789, 588-594.	5.5	7
18	Unraveling the Degradation Mechanism of FIrpic-Based Blue OLEDs: I. A Theoretical Investigation. Chemistry of Materials, 2019, 31, 2269-2276.	6.7	9

#	Article	IF	Citations
19	Unraveling the Degradation Mechanism in FIrpic-Based Blue OLEDs: II. Trap and Detect Molecules at the Interfaces. Chemistry of Materials, 2019, 31, 2277-2285.	6.7	27
20	Tailoring topological states in silicene using different halogen-passivated Si(111) substrates. Physical Review B, 2018, 97, .	3.2	2
21	Magnetic Moments and Electron Transport through Chromium-Based Antiferromagnetic Nanojunctions. Materials, 2018, 11, 2030.	2.9	3
22	Rare Earth Doped Ceria: The Complex Connection Between Structure and Properties. Frontiers in Chemistry, 2018, 6, 526.	3.6	88
23	Vibrational and thermoelastic properties of bcc iron from selected EAM potentials. Computational Materials Science, 2018, 152, 99-106.	3.0	8
24	Î²-Diketonate ancillary ligands in heteroleptic iridium complexes: a balance between synthetic advantages and photophysical troubles. Photochemical and Photobiological Sciences, 2018, 17, 1169-1178.	2.9	6
25	Ï€â€“Ï€-Induced aggregation and single-crystal fluorescence anisotropy of 5,6,10b-triazaacephenanthrylene. IUCrJ, 2018, 5, 335-347.	2.2	10
26	A polynomial Ansatz for norm-conserving pseudopotentials. Journal of Physics Condensed Matter, 2018, 30, 275501.	1.8	0
27	Experimental evidence for pressure-induced first order transition in cerium nitride from B1 to B10 structure type. Journal of Applied Physics, 2017, 121, .	2.5	14
28	DFT investigation of the effect of spin-orbit coupling on the NMR shifts in paramagnetic solids. Physical Review B, 2017, 95, .	3.2	31
29	eQE: An openâ€source density functional embedding theory code for the condensed phase. International Journal of Quantum Chemistry, 2017, 117, e25401.	2.0	40
30	Upper limit to the ultimate achievable emission wavelength in near-IR emitting cyclometalated iridium complexes. Photochemical and Photobiological Sciences, 2017, 16, 1220-1223.	2.9	17
31	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
32	Elastic constants and mechanical properties of PEDOT from first principles calculations. Computational Materials Science, 2017, 139, 234-242.	3.0	15
33	AFLOWÏ€: A minimalist approach to high-throughput ab initio calculations including the generation of tight-binding hamiltonians. Computational Materials Science, 2017, 136, 76-84.	3.0	70
34	High-pressure phase diagram, structural transitions, and persistent nonmetallicity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaBiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m : Theory and experiment. Physical Review Materials, 2017, 1, .	2.4	3
35	Avoiding fractional electrons in subsystem DFT based ab-initio molecular dynamics yields accurate models for liquid water and solvated OH radical. Journal of Chemical Physics, 2016, 144, 234105.	3.0	28
36	Quantum mechanical calculation of Rydbergâ€“Rydberg autoionization rates. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 204004.	1.5	12

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37	Spin-filtering in graphene junctions with Ti and Co adsorbates. Chemical Physics, 2016, 478, 91-96.	1.9	5
38	Source function and plane waves: Toward complete bader analysis. Journal of Computational Chemistry, 2016, 37, 2133-2139.	3.3	8
39	Accurate tight-binding Hamiltonians for two-dimensional and layered materials. Physical Review B, 2016, 93, .	3.2	40
40	Electronic transport in B-N substituted bilayer graphene nanojunctions. Physical Review B, 2016, 93, .	3.2	8
41	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.	13.8	126
42	Nearâ€IR Emitting Iridium(III) Complexes with Heteroaromatic Î²â€Diketonate Ancillary Ligands for Efficient Solutionâ€Processed OLEDs: Structureâ€“Property Correlations. Angewandte Chemie, 2016, 128, 2764-2768.	2.0	23
43	Exploiting the Photonic Crystal Properties of TiO₂ Nanotube Arrays To Enhance Photocatalytic Hydrogen Production. ACS Catalysis, 2016, 6, 1345-1353.	11.2	117
44	Spin diffusion in the low-dimensional molecular quantum Heisenberg antiferromagnet<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Cu</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:m with implanted muons. Physical Review B, 2015, 91, .	3.2	28
45	High-pressure synthesis of bismuth disulfide, structural solution and its physical properties. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s79-s79.	0.1	0
46	Thermoelastic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math>-iron from first-principles. Physical Review B, 2015, 91, .	3.2	40
47	Subsystem real-time time dependent density functional theory. Journal of Chemical Physics, 2015, 142, 154116.	3.0	34
48	Phase stability of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrMn</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>hexagonal perovskite system at high pressure and temperature. Physical Review B, 2014, 90, .	3.2	29
49	Periodic subsystem density-functional theory. Journal of Chemical Physics, 2014, 141, 174101.	3.0	42
50	NCImilano: an electron-density-based code for the study of noncovalent interactions. Journal of Applied Crystallography, 2013, 46, 1513-1517.	4.5	50
51	Enhancement of DFT-calculations at petascale: Nuclear Magnetic Resonance, Hybrid Density Functional Theory and Carâ€“Parrinello calculations. Computer Physics Communications, 2013, 184, 1827-1833.	7.5	33
52	Quantum states of muons in fluorides. Physical Review B, 2013, 87, .	3.2	57
53	Playing quantum hide-and-seek with the muon: localizing muon stopping sites. Physica Scripta, 2013, 88, 068510.	2.5	67
54	An integrated framework for multi-scale multi-physics numerical modelling of interface evolution in welding. IOP Conference Series: Materials Science and Engineering, 2012, 33, 012029.	0.6	5

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55	First-principles investigation of hyperfine interactions for nuclear spin entanglement in photoexcited fullerenes. Physical Review B, 2012, 85, .	3.2	9
56	Effect of pressure on the energy band gaps of wurtzite GaN and AlN and electronic properties of their ternary alloys AlxGa1â^'xN. Physica B: Condensed Matter, 2012, 407, 3604-3609.	2.7	8
57	First principles NMR study of fluorapatite under pressure. Solid State Nuclear Magnetic Resonance, 2012, 45-46, 59-65.	2.3	12
58	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Si</mml:mtext></mml:mrow><mml:mtext>C</mml:mtext></mml pairs in SiC identified as paramagnetic defects with strongly anisotropic orbital quenching. Physical Review B, 2010, 81, .	3.2	15
59	First-principles theory of orbital magnetization. Physical Review B, 2010, 81, .	3.2	77
60	Ab initioconverse NMR approach for pseudopotentials. Physical Review B, 2010, 81, .	3.2	25
61	NMR shifts for polycyclic aromatic hydrocarbons from firstâ€principles. International Journal of Quantum Chemistry, 2009, 109, 3336-3342.	2.0	39
62	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	1.8	18,183
63	A converse approach to the calculation of NMR shielding tensors. Journal of Chemical Physics, 2009, 131, 101101.	3.0	54
64	Alkali halide surfaces near melting: Wetting and nanofriction properties. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2008, 495, 32-35.	5.6	1
65	Charging induced emission of neutral atoms from NaCl nanocube corners. Journal of Physics Condensed Matter, 2008, 20, 325236.	1.8	1
66	Electron-corrected Lorentz forces in solids and molecules in a magnetic field. Physical Review B, 2007, 75, .	3.2	17
67	Orbital magnetization and Chern number in a supercell framework: Single<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi mathvariant="bold">k</mml:mi></mml:math>-point formula. Physical Review B, 2007, 76, .	3.2	20
68	Peak effect versus skating in high-temperature nanofriction. Nature Materials, 2007, 6, 230-234.	27.5	30
69	Orbital magnetization in crystalline solids: Multi-band insulators, Chern insulators, and metals. Physical Review B, 2006, 74, .	3.2	218
70	Structural and dielectric properties of amorphousZrO2andHfO2. Physical Review B, 2006, 74, .	3.2	148
71	Electron-stimulated emission of Na atoms from NaCl nanocube corners. Surface Science, 2006, 600, 4315-4318.	1.9	1
72	Physics and nanofriction of alkali halide solid surfaces at the melting point. Surface Science, 2006, 600, 4395-4398.	1.9	1

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73	Structural and dielectric properties of crystalline and amorphous ZrO2. Thin Solid Films, 2005, 486, 125-128.	1.8	160
74	Orbital Magnetization in Extended Systems. ChemPhysChem, 2005, 6, 1815-1819.	2.1	28
75	Why Are Alkali Halide Surfaces Not Wetted by Their Own Melt?. Physical Review Letters, 2005, 94, 176105.	7.8	40
76	Exciton self-trapping in bulk polyethylene. Journal of Physics Condensed Matter, 2005, 17, 4621-4627.	1.8	27
77	Physics of solid and liquid alkali halide surfaces near the melting point. Journal of Chemical Physics, 2005, 123, 164701.	3.0	31
78	Structural, electronic, and dielectric properties of amorphousZrO2fromab initiomolecular dynamics. Physical Review B, 2005, 71, .	3.2	135
79	Orbital Magnetization in Periodic Insulators. Physical Review Letters, 2005, 95, 137205.	7.8	300
80	Trapping of excitons at chemical defects in polyethylene. Journal of Chemical Physics, 2004, 121, 6478-6484.	3.0	39
81	NaCl nanodroplet on NaCl(100) at the melting point. Surface Science, 2004, 566-568, 794-798.	1.9	14
82	Berry-Phase Calculation of Magnetic Screening and RotationalgFactor in Molecules and Solids. Physical Review Letters, 2002, 89, 116402.	7.8	13
83	Dehydroxylation and Silanization of the Surfaces of Î²-Cristobalite Silica:Â An ab Initio Simulation. Journal of Physical Chemistry B, 2001, 105, 8007-8013.	2.6	95
84	Two-Membered Silicon Rings on the Dehydroxylated Surface of Silica. Physical Review Letters, 2000, 84, 3887-3890.	7.8	150