# 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 | 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 |
| 2 | Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901. | 1.8 | 4,303 |
| 3 | Orbital Magnetization in Periodic Insulators. Physical Review Letters, 2005, 95, 137205. | 7.8 | 300 |
| 4 | Orbital magnetization in crystalline solids: Multi-band insulators, Chern insulators, and metals. Physical Review B, 2006, 74, . | 3.2 | 218 |
| 5 | Structural and dielectric properties of crystalline and amorphous ZrO2. Thin Solid Films, 2005, 486, 125-128. | 1.8 | 160 |
| 6 | Two-Membered Silicon Rings on the Dehydroxylated Surface of Silica. Physical Review Letters, 2000, 84, 3887-3890. | 7.8 | 150 |
| 7 | Structural and dielectric properties of amorphousZrO2andHfO2. Physical Review B, 2006, 74, . | 3.2 | 148 |
| 8 | Structural, electronic, and dielectric properties of amorphousZrO2fromab initiomolecular dynamics. Physical Review B, 2005, 71, . | 3.2 | 135 |
| 9 | 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 |
| 10 | Exploiting the Photonic Crystal Properties of TiO<sub>2</sub> Nanotube Arrays To Enhance Photocatalytic Hydrogen Production. ACS Catalysis, 2016, 6, 1345-1353. | 11.2 | 117 |
| 11 | 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 |
| 12 | Rare Earth Doped Ceria: The Complex Connection Between Structure and Properties. Frontiers in Chemistry, 2018, 6, 526. | 3.6 | 88 |
| 13 | First-principles theory of orbital magnetization. Physical Review B, 2010, 81, . | 3.2 | 77 |
| 14 | 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 |
| 15 | Playing quantum hide-and-seek with the muon: localizing muon stopping sites. Physica Scripta, 2013, 88, 068510. | 2.5 | 67 |
| 16 | Quantum states of muons in fluorides. Physical Review B, 2013, 87, . | 3.2 | 57 |
| 17 | A converse approach to the calculation of NMR shielding tensors. Journal of Chemical Physics, 2009, 131, 101101. | 3.0 | 54 |
| 18 | NCImilano: an electron-density-based code for the study of noncovalent interactions. Journal of Applied Crystallography, 2013, 46, 1513-1517. | 4.5 | 50 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Periodic subsystem density-functional theory. Journal of Chemical Physics, 2014, 141, 174101. | 3.0 | 42 |
| 20 | Why Are Alkali Halide Surfaces Not Wetted by Their Own Melt?. Physical Review Letters, 2005, 94, 176105. | 7.8 | 40 |
| 21 | 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 |
| 22 | Accurate tight-binding Hamiltonians for two-dimensional and layered materials. Physical Review B, 2016, 93, . | 3.2 | 40 |
| 23 | eQE: An openâ€source density functional embedding theory code for the condensed phase. International Journal of Quantum Chemistry, 2017, 117, e25401. | 2.0 | 40 |
| 24 | Trapping of excitons at chemical defects in polyethylene. Journal of Chemical Physics, 2004, 121, 6478-6484. | 3.0 | 39 |
| 25 | NMR shifts for polycyclic aromatic hydrocarbons from firstâ€principles. International Journal of Quantum Chemistry, 2009, 109, 3336-3342. | 2.0 | 39 |
| 26 | Local Structure and Magnetism of Fe2O3 Maghemite Nanocrystals: The Role of Crystal Dimension. Nanomaterials, 2020, 10, 867. | 4.1 | 37 |
| 27 | Subsystem real-time time dependent density functional theory. Journal of Chemical Physics, 2015, 142, 154116. | 3.0 | 34 |
| 28 | 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 |
| 29 | Physics of solid and liquid alkali halide surfaces near the melting point. Journal of Chemical Physics, 2005, 123, 164701. | 3.0 | 31 |
| 30 | DFT investigation of the effect of spin-orbit coupling on the NMR shifts in paramagnetic solids. Physical Review B, 2017, 95, . | 3.2 | 31 |
| 31 | Peak effect versus skating in high-temperature nanofriction. Nature Materials, 2007, 6, 230-234. | 27.5 | 30 |
| 32 | 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 |
| 33 | Orbital Magnetization in Extended Systems. ChemPhysChem, 2005, 6, 1815-1819. | 2.1 | 28 |
| 34 | 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:mrow><mml:mn> with implanted muons. Physical Review B, 2015, 91, . | 3.2 | 28 |
| 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 | Exciton self-trapping in bulk polyethylene. Journal of Physics Condensed Matter, 2005, 17, 4621-4627. | 1.8 | 27 |

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| 37 | 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 |
| 38 | Ab initioconverse NMR approach for pseudopotentials. Physical Review B, 2010, 81, . | 3.2 | 25 |
| 39 | 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 |
| 40 | Advanced modeling of materials with PAOFLOW 2.0: New features and software design. Computational Materials Science, 2021, 200, 110828. | 3.0 | 21 |
| 41 | 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 |
| 42 | 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 |
| 43 | Electron-corrected Lorentz forces in solids and molecules in a magnetic field. Physical Review B, 2007, 75, . | 3.2 | 17 |
| 44 | 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 |
| 45 | <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:m pairs in SiC identified as paramagnetic defects with strongly anisotropic orbital quenching. Physical Review B, 2010, 81, . | 3.2 | 15 |
| 46 | Elastic constants and mechanical properties of PEDOT from first principles calculations. Computational Materials Science, 2017, 139, 234-242. | 3.0 | 15 |
| 47 | NaCl nanodroplet on NaCl(100) at the melting point. Surface Science, 2004, 566-568, 794-798. | 1.9 | 14 |
| 48 | 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 |
| 49 | Berry-Phase Calculation of Magnetic Screening and RotationalgFactor in Molecules and Solids. Physical Review Letters, 2002, 89, 116402. | 7.8 | 13 |
| 50 | eQE 2.0: Subsystem DFT beyond GGA functionals. Computer Physics Communications, 2021, 269, 108122. | 7.5 | 13 |
| 51 | First principles NMR study of fluorapatite under pressure. Solid State Nuclear Magnetic Resonance, 2012, 45-46, 59-65. | 2.3 | 12 |
| 52 | Quantum mechanical calculation of Rydbergâ€“Rydberg autoionization rates. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 204004. | 1.5 | 12 |
| 53 | Ï€â€“Ï€-Induced aggregation and single-crystal fluorescence anisotropy of 5,6,10b-triazaacephenanthrylene. IUCrJ, 2018, 5, 335-347. | 2.2 | 10 |
| 54 | First-principles investigation of hyperfine interactions for nuclear spin entanglement in photoexcited fullerenes. Physical Review B, 2012, 85, . | 3.2 | 9 |

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| 55 | Unraveling the Degradation Mechanism of FIrpic-Based Blue OLEDs: I. A Theoretical Investigation. Chemistry of Materials, 2019, 31, 2269-2276. | 6.7 | 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 | Source function and plane waves: Toward complete bader analysis. Journal of Computational Chemistry, 2016, 37, 2133-2139. | 3.3 | 8 |
| 58 | Electronic transport in B-N substituted bilayer graphene nanojunctions. Physical Review B, 2016, 93, . | 3.2 | 8 |
| 59 | Vibrational and thermoelastic properties of bcc iron from selected EAM potentials. Computational Materials Science, 2018, 152, 99-106. | 3.0 | 8 |
| 60 | 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 | 8 |
| 61 | 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 |
| 62 | 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 |
| 63 | First-principles evaluation of the secondary electron yield (Î³<sup> N </sup>) from polyethylene surface. Journal Physics D: Applied Physics, 2020, 53, 175301. | 2.8 | 6 |
| 64 | Electronic structure of defected polyethylene for Schottky emission. Materials Chemistry and Physics, 2021, 263, 124268. | 4.0 | 6 |
| 65 | 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 |
| 66 | Spin-filtering in graphene junctions with Ti and Co adsorbates. Chemical Physics, 2016, 478, 91-96. | 1.9 | 5 |
| 67 | 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 |
| 68 | High-Pressure Computational Search of Trivalent Lanthanide Dinitrides. Journal of Physical Chemistry C, 2021, 125, 161-167. | 3.1 | 5 |
| 69 | GIPAW Pseudopotentials of d Elements for Solid-State NMR. Materials, 2022, 15, 3347. | 2.9 | 4 |
| 70 | Magnetic Moments and Electron Transport through Chromium-Based Antiferromagnetic Nanojunctions. Materials, 2018, 11, 2030. | 2.9 | 3 |
| 71 | High pressure structure studies of three SrGeO3 polymorphs â€“ Amorphization under pressure. Journal of Alloys and Compounds, 2021, 855, 157419. | 5.5 | 3 |
| 72 | About the deterioration of polyethylene exposed to plasma discharges: A comparison between two models. Applied Surface Science, 2021, 567, 150306. | 6.1 | 3 |

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| 73 | Tailoring topological states in silicene using different halogen-passivated Si(111) substrates. Physical Review B, 2018, 97, . | 3.2 | 2 |
| 74 | 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 |
| 75 | 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 |
| 76 | 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 |
| 77 | Electron-stimulated emission of Na atoms from NaCl nanocube corners. Surface Science, 2006, 600, 4315-4318. | 1.9 | 1 |
| 78 | Physics and nanofriction of alkali halide solid surfaces at the melting point. Surface Science, 2006, 600, 4395-4398. | 1.9 | 1 |
| 79 | 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 |
| 80 | Charging induced emission of neutral atoms from NaCl nanocube corners. Journal of Physics Condensed Matter, 2008, 20, 325236. | 1.8 | 1 |
| 81 | 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 |
| 82 | 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 |
| 83 | A polynomial Ansatz for norm-conserving pseudopotentials. Journal of Physics Condensed Matter, 2018, 30, 275501. | 1.8 | 0 |
| 84 | Anharmonic motion and aspherical nuclear probability density functions in cesium halides. Physical Review B, 2022, 105, . | 3.2 | 0 |