Asstâ€prof Ivano E Castelli

List of Publications by Year
in descending order

83 papers	8,910 citations	136950 32 h-index	58581 82 g-index
94 all docs	94 docs citations	94 times ranked	12869 citing authors

#	Article	IF	Citations
1	Bandgap prediction of metal halide perovskites using regression machine learning models. Physics Letters, Section A: General, Atomic and Solid State Physics, 2022, 422, 127800.	2.1	29
2	A Roadmap for Transforming Research to Invent the Batteries of the Future Designed within the European Large Scale Research Initiative BATTERY 2030+. Advanced Energy Materials, 2022, 12, .	19.5	70
3	Autonomous Design of Photoferroic Ruddlesden-Popper Perovskites for Water Splitting Devices. Materials, 2022, 15, 309.	2.9	3
4	Optimizing the quasi-equilibrium state of hot carriers in all-inorganic lead halide perovskite nanocrystals through Mn doping: fundamental dynamics and device perspectives. Chemical Science, 2022, 13, 1734-1745.	7.4	11
5	Towards autonomous high-throughput multiscale modelling of battery interfaces. Energy and Environmental Science, 2022, 15, 579-594.	30.8	17
6	On the thermoelectric properties of Nb-doped SrTiO₃ epitaxial thin films. Physical Chemistry Chemical Physics, 2022, 24, 3741-3748.	2.8	9
7	Workflow Engineering in Materials Design within the BATTERY 2030+ Project. Advanced Energy Materials, 2022, 12, .	19.5	18
8	Rechargeable Batteries of the Futureâ€"The State of the Art from a BATTERY 2030+ Perspective. Advanced Energy Materials, 2022, 12, .	19.5	124
9	Understanding Battery Interfaces by Combined Characterization and Simulation Approaches: Challenges and Perspectives. Advanced Energy Materials, 2022, 12, .	19.5	46
10	Editorial to the Special Issue: How to Reinvent the Ways to Invent the Batteries of the Future â€“ the Battery 2030+ Largeâ€Scale Research Initiative Roadmap. Advanced Energy Materials, 2022, 12, .	19.5	6
11	Nanotubes from Ternary WS_{2(1â€“x)}Se_{2x} Alloys: Stoichiometry Modulated Tunable Optical Properties. Journal of the American Chemical Society, 2022, 144, 10530-10542.	13.7	15
12	Observation of Biradical Spin Coupling through Hydrogen Bonds. Physical Review Letters, 2022, 128, .	7.8	6
13	Synergistic effects in oxygen evolution activity of mixed iridium-ruthenium pyrochlores. Electrochimica Acta, 2021, 366, 137327.	5.2	17
14	Oxygen evolution reaction activity and underlying mechanism of perovskite electrocatalysts at different pH. Materials Advances, 2021, 2, 345-355.	5.4	42
15	Electromechanically active pair dynamics in a Gd-doped ceria single crystal. Physical Chemistry Chemical Physics, 2021, 23, 11233-11239.	2.8	5
16	Exploring the Intrinsic Point Defects in Cesium Copper Halides. Journal of Physical Chemistry C, 2021, 125, 1592-1598.	3.1	15
17	Structural and chemical mechanisms governing stability of inorganic Janus nanotubes. Npj Computational Materials, 2021, 7, .	8.7	22
18	Nonlinear Photoelectric Properties by Strained MoS₂ and SnO₂ Coreâ€Shell Nanotubes for Flexible Visible Light Photodetectors. Advanced Materials Technologies, 2021, 6, 2001105.	5.8	4

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19	Theoretical Insight on Anion Ordering, Strain, and Doping Engineering of the Oxygen Evolution Reaction in BaTaO2N. Chemistry of Materials, 2021, 33, 3297-3303.	6.7	15
20	Atomic-Scale Observation of Oxygen Vacancy-Induced Step Reconstruction in WO₃. Journal of Physical Chemistry C, 2021, 125, 8456-8460.	3.1	6
21	Free Carriers versus Self-Trapped Excitons at Different Facets of Ruddlesdenâ€“Popper Two-Dimensional Lead Halide Perovskite Single Crystals. Journal of Physical Chemistry Letters, 2021, 12, 4965-4971.	4.6	27
22	Automatic Migration Path Exploration for Multivalent Battery Cathodes using Geometrical Descriptors. Batteries and Supercaps, 2021, 4, 1516-1524.	4.7	11
23	Data Management Plans: the Importance of Data Management in the BIGâ€MAP Project**. Batteries and Supercaps, 2021, 4, 1803-1812.	4.7	19
24	Enhancing Oxygen Evolution Reaction Activity by Using Switchable Polarization in Ferroelectric InSnO₂N. ACS Catalysis, 2021, 11, 12692-12700.	11.2	9
25	Band structure of MoSTe Janus nanotubes. Physical Review Materials, 2021, 5, .	2.4	23
26	Influence of the Artificial Nanostructure on the LiF Formation at the Solidâ€“Electrolyte Interphase of Carbon-Based Anodes. ACS Applied Energy Materials, 2021, 4, 35-41.	5.1	2
27	Towards photoferroic materials by design: recent progress and perspectives. JPhys Energy, 2020, 2, 011001.	5.3	13
28	Atomic-scale insights into electro-steric substitutional chemistry of cerium oxide. Physical Chemistry Chemical Physics, 2020, 22, 21900-21908.	2.8	6
29	Metastability at Defective Metal Oxide Interfaces and Nanoconfined Structures. Advanced Materials Interfaces, 2020, 7, 1902090.	3.7	20
30	The role of an interface in stabilizing reaction intermediates for hydrogen evolution in aprotic electrolytes. Chemical Science, 2020, 11, 3914-3922.	7.4	23
31	Autonomous Discovery of Materials for Intercalation Electrodes. Batteries and Supercaps, 2020, 3, 473-473.	4.7	0
32	Effect of high oxygen deficiency in nano-confined bismuth sesquioxide. JPhys Energy, 2020, 2, 024010.	5.3	1
33	Autonomous Discovery of Materials for Intercalation Electrodes. Batteries and Supercaps, 2020, 3, 488-498.	4.7	25
34	Modulating Charge-Carrier Dynamics in Mn-Doped All-Inorganic Halide Perovskite Quantum Dots through the Doping-Induced Deep Trap States. Journal of Physical Chemistry Letters, 2020, 11, 3705-3711.	4.6	22
35	Electronic Structure and Trap States of Two-Dimensional Ruddlesdenâ€“Popper Perovskites with the Relaxed Goldschmidt Tolerance Factor. ACS Applied Electronic Materials, 2020, 2, 1402-1412.	4.3	19
36	Machine-learning structural and electronic properties of metal halide perovskites using a hierarchical convolutional neural network. Npj Computational Materials, 2020, 6, .	8.7	93

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37	Air Stable, Highâ€Efficiency, Ptâ€Based Halide Perovskite Solar Cells with Long Carrier Lifetimes. Physica Status Solidi - Rapid Research Letters, 2020, 14, 2000182.	2.4	39
38	Fundamental Atomic Insight in Electrocatalysis. , 2020, , 1473-1503.		1
39	Design and Synthesis of Ir/Ru Pyrochlore Catalysts for the Oxygen Evolution Reaction Based on Their Bulk Thermodynamic Properties. ACS Applied Materials & Interfaces, 2019, 11, 37748-37760.	8.0	61
40	Yttrium Tantalum Oxynitride Multiphases as Photoanodes for Water Oxidation. Journal of Physical Chemistry C, 2019, 123, 26211-26217.	3.1	9
41	A perspective on inverse design of battery interphases using multi-scale modelling, experiments and generative deep learning. Energy Storage Materials, 2019, 21, 446-456.	18.0	79
42	Fe-Doping in Double Perovskite PrBaCo2(1-x)Fe2xO6-Î´: Insights into Structural and Electronic Effects to Enhance Oxygen Evolution Catalyst Stability. Catalysts, 2019, 9, 263.	3.5	25
43	Functional Role of Fe-Doping in Co-Based Perovskite Oxide Catalysts for Oxygen Evolution Reaction. Journal of the American Chemical Society, 2019, 141, 5231-5240.	13.7	250
44	High-Entropy Alloys as a Discovery Platform for Electrocatalysis. Joule, 2019, 3, 834-845.	24.0	464
45	Electrocatalytic transformation of HF impurity to H2 and LiF in lithium-ion batteries. Nature Catalysis, 2018, 1, 255-262.	34.4	128
46	Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. Nature Nanotechnology, 2018, 13, 246-252.	31.5	1,317
47	Oxidation of Ethylene Carbonate on Li Metal Oxide Surfaces. Journal of Physical Chemistry C, 2018, 122, 10442-10449.	3.1	60
48	Precision and efficiency in solid-state pseudopotential calculations. Npj Computational Materials, 2018, 4, .	8.7	390
49	Highly Active Nanoperovskite Catalysts for Oxygen Evolution Reaction: Insights into Activity and Stability of Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{2+Î´} and PrBaCo₂O_{5+Î´}. Advanced Functional Materials, 2018, 28, 1804355.	14.9	63
50	Oxygen Evolution Reaction on Perovskites: A Multieffect Descriptor Study Combining Experimental and Theoretical Methods. ACS Catalysis, 2018, 8, 9567-9578.	11.2	98
51	Effects of the cooperative interaction on the diffusion of hydrogen on MgO(100). Journal of Chemical Physics, 2018, 149, 034704.	3.0	10
52	Fundamental Atomic Insight in Electrocatalysis. , 2018, , 1-31.		4
53	Chapter 3. Computational Screening of Light-absorbing Materials for Photoelectrochemical Water Splitting. RSC Energy and Environment Series, 2018, , 62-99.	0.5	2
54	Role of Fe-Doping in Perovskite Oxides for the Oxygen Evolution Reaction. ECS Meeting Abstracts, 2018, , .	0.0	0

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55	Synergetic Surface Sensitivity of Photoelectrochemical Water Oxidation on TiO₂ (Anatase) Electrodes. Journal of Physical Chemistry C, 2017, 121, 6024-6032.	3.1	18
56	Highly Active and Stable Iridium Pyrochlores for Oxygen Evolution Reaction. Chemistry of Materials, 2017, 29, 5182-5191.	6.7	172
57	Determination of Conduction and Valence Band Electronic Structure of LaTiO x N y Thin Film. ChemSusChem, 2017, 10, 2099-2106.	6.8	19
58	The atomic simulation environmentâ€”a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	1.8	1,933
59	Unraveling Thermodynamics, Stability, and Oxygen Evolution Activity of Strontium Ruthenium Perovskite Oxide. ACS Catalysis, 2017, 7, 3245-3256.	11.2	113
60	Anisotropic Proton and Oxygen Ion Conductivity in Epitaxial Ba2In2O5 Thin Films. Journal of Physical Chemistry C, 2017, 121, 21797-21805.	3.1	16
61	Role of the Band Gap for the Interaction Energy of Coadsorbed Fragments. Journal of Physical Chemistry C, 2017, 121, 18608-18614.	3.1	15
62	Defect Chemistry and Electrical Conductivity of Sm-Doped La_{1â€“x}Sr_xCoO_{3â^'Î´} for Solid Oxide Fuel Cells. Journal of Physical Chemistry C, 2017, 121, 15017-15027.	3.1	13
63	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
64	Band-gap engineering of functional perovskites through quantum confinement and tunneling. Physical Review B, 2015, 91, .	3.2	13
65	Strain sensitivity of band gaps of Sn-containing semiconductors. Physical Review B, 2015, 91, .	3.2	24
66	Calculated optical absorption of different perovskite phases. Journal of Materials Chemistry A, 2015, 3, 12343-12349.	10.3	35
67	Oxygen Evolution Reaction on La_{1â€“x}Sr_xCoO₃ Perovskites: A Combined Experimental and Theoretical Study of Their Structural, Electronic, and Electrochemical Properties. Chemistry of Materials, 2015, 27, 7662-7672.	6.7	259
68	New Lightâ€Harvesting Materials Using Accurate and Efficient Bandgap Calculations. Advanced Energy Materials, 2015, 5, 1400915.	19.5	124
69	Designing rules and probabilistic weighting for fast materials discovery in the Perovskite structure. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 055007.	2.0	24
70	Bandgap calculations and trends of organometal halide perovskites. APL Materials, 2014, 2, .	5.1	222
71	Calculated Pourbaix Diagrams of Cubic Perovskites for Water Splitting: Stability Against Corrosion. Topics in Catalysis, 2014, 57, 265-272.	2.8	47
72	2-Photon tandem device for water splitting: comparing photocathode first versus photoanode first designs. Energy and Environmental Science, 2014, 7, 2397-2413.	30.8	130

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73	Performance of genetic algorithms in search for water splitting perovskites. Journal of Materials Science, 2013, 48, 6519-6534.	3.7	42
74	Stability and bandgaps of layered perovskites for one- and two-photon water splitting. New Journal of Physics, 2013, 15, 105026.	2.9	51
75	Bandgap Engineering of Double Perovskites for One- and Two-photon Water Splitting. Materials Research Society Symposia Proceedings, 2013, 1523, 601.	0.1	13
76	Computational screening of perovskite metal oxides for optimal solar light capture. Energy and Environmental Science, 2012, 5, 5814-5819.	30.8	354
77	Mechanical properties of carbynes investigated byab initiototal-energy calculations. Physical Review B, 2012, 85, .	3.2	41
78	New cubic perovskites for one- and two-photon water splitting using the computational materials repository. Energy and Environmental Science, 2012, 5, 9034.	30.8	211
79	Carbon sp chains in graphene nanoholes. Journal of Physics Condensed Matter, 2012, 24, 104019.	1.8	15
80	Vibrational characterization of dinaphthylpolyynes: A model system for the study of end-capped sp carbon chains. Journal of Chemical Physics, 2011, 135, 194501.	3.0	21
81	Synthesis, Characterization, and Modeling of Naphthyl-Terminated sp Carbon Chains: Dinaphthylpolyynes. Journal of Physical Chemistry B, 2010, 114, 14834-14841.	2.6	45
82	Tribology of the lubricant quantized sliding state. Journal of Chemical Physics, 2009, 131, 174711.	3.0	13
83	Role of transverse displacements for a quantized-velocity state of a lubricant. Journal of Physics Condensed Matter, 2008, 20, 354005.	1.8	12