

# Asstâ€™prof Ivano E Castelli

## List of Publications by Year in descending order

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Version: 2024-02-01

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	The atomic simulation environment—a Python library for working with atoms. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 273002.	1.8	1,933
2	Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds. <i>Nature Nanotechnology</i> , 2018, 13, 246-252.	31.5	1,317
3	Reproducibility in density functional theory calculations of solids. <i>Science</i> , 2016, 351, aad3000.	12.6	1,113
4	High-Entropy Alloys as a Discovery Platform for Electrocatalysis. <i>Joule</i> , 2019, 3, 834-845.	24.0	464
5	Precision and efficiency in solid-state pseudopotential calculations. <i>Npj Computational Materials</i> , 2018, 4, .	8.7	390
6	Computational screening of perovskite metal oxides for optimal solar light capture. <i>Energy and Environmental Science</i> , 2012, 5, 5814-5819.	30.8	354
7	Oxygen Evolution Reaction on La <sub>1-x</sub> Sr <sub>x</sub> CoO <sub>3</sub> Perovskites: A Combined Experimental and Theoretical Study of Their Structural, Electronic, and Electrochemical Properties. <i>Chemistry of Materials</i> , 2015, 27, 7662-7672.	6.7	259
8	Functional Role of Fe-Doping in Co-Based Perovskite Oxide Catalysts for Oxygen Evolution Reaction. <i>Journal of the American Chemical Society</i> , 2019, 141, 5231-5240.	13.7	250
9	Bandgap calculations and trends of organometal halide perovskites. <i>APL Materials</i> , 2014, 2, .	5.1	222
10	New cubic perovskites for one- and two-photon water splitting using the computational materials repository. <i>Energy and Environmental Science</i> , 2012, 5, 9034.	30.8	211
11	Highly Active and Stable Iridium Pyrochlores for Oxygen Evolution Reaction. <i>Chemistry of Materials</i> , 2017, 29, 5182-5191.	6.7	172
12	2-Photon tandem device for water splitting: comparing photocathode first versus photoanode first designs. <i>Energy and Environmental Science</i> , 2014, 7, 2397-2413.	30.8	130
13	Electrocatalytic transformation of HF impurity to H <sub>2</sub> and LiF in lithium-ion batteries. <i>Nature Catalysis</i> , 2018, 1, 255-262.	34.4	128
14	New Light-Harvesting Materials Using Accurate and Efficient Bandgap Calculations. <i>Advanced Energy Materials</i> , 2015, 5, 1400915.	19.5	124
15	Rechargeable Batteries of the Future—The State of the Art from a BATTERY 2030+ Perspective. <i>Advanced Energy Materials</i> , 2022, 12, .	19.5	124
16	Unraveling Thermodynamics, Stability, and Oxygen Evolution Activity of Strontium Ruthenium Perovskite Oxide. <i>ACS Catalysis</i> , 2017, 7, 3245-3256.	11.2	113
17	Oxygen Evolution Reaction on Perovskites: A Multieffect Descriptor Study Combining Experimental and Theoretical Methods. <i>ACS Catalysis</i> , 2018, 8, 9567-9578.	11.2	98
18	Machine-learning structural and electronic properties of metal halide perovskites using a hierarchical convolutional neural network. <i>Npj Computational Materials</i> , 2020, 6, .	8.7	93

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19	A perspective on inverse design of battery interphases using multi-scale modelling, experiments and generative deep learning. <i>Energy Storage Materials</i> , 2019, 21, 446-456.	18.0	79
20	A Roadmap for Transforming Research to Invent the Batteries of the Future Designed within the European Large Scale Research Initiative BATTERY 2030+. <i>Advanced Energy Materials</i> , 2022, 12, .	19.5	70
21	Highly Active Nanoperovskite Catalysts for Oxygen Evolution Reaction: Insights into Activity and Stability of $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{Co}_{0.8}\text{Fe}_{0.2}\text{O}_{2+\delta}$ and $\text{PrBaCo}_2\text{O}_{5+\delta}$ . <i>Advanced Functional Materials</i> , 2018, 28, 1804355.	14.9	63
22	Design and Synthesis of Ir/Ru Pyrochlore Catalysts for the Oxygen Evolution Reaction Based on Their Bulk Thermodynamic Properties. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 37748-37760.	8.0	61
23	Oxidation of Ethylene Carbonate on Li Metal Oxide Surfaces. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10442-10449.	3.1	60
24	Stability and bandgaps of layered perovskites for one- and two-photon water splitting. <i>New Journal of Physics</i> , 2013, 15, 105026.	2.9	51
25	Calculated Pourbaix Diagrams of Cubic Perovskites for Water Splitting: Stability Against Corrosion. <i>Topics in Catalysis</i> , 2014, 57, 265-272.	2.8	47
26	Understanding Battery Interfaces by Combined Characterization and Simulation Approaches: Challenges and Perspectives. <i>Advanced Energy Materials</i> , 2022, 12, .	19.5	46
27	Synthesis, Characterization, and Modeling of Naphthyl-Terminated sp Carbon Chains: Dinaphthylpolyynes. <i>Journal of Physical Chemistry B</i> , 2010, 114, 14834-14841.	2.6	45
28	Performance of genetic algorithms in search for water splitting perovskites. <i>Journal of Materials Science</i> , 2013, 48, 6519-6534.	3.7	42
29	Oxygen evolution reaction activity and underlying mechanism of perovskite electrocatalysts at different pH. <i>Materials Advances</i> , 2021, 2, 345-355.	5.4	42
30	Mechanical properties of carbynes investigated by ab initio total-energy calculations. <i>Physical Review B</i> , 2012, 85, .	3.2	41
31	Air Stable, High Efficiency, Pt-Free Based Halide Perovskite Solar Cells with Long Carrier Lifetimes. <i>Physica Status Solidi - Rapid Research Letters</i> , 2020, 14, 2000182.	2.4	39
32	Calculated optical absorption of different perovskite phases. <i>Journal of Materials Chemistry A</i> , 2015, 3, 12343-12349.	10.3	35
33	Bandgap prediction of metal halide perovskites using regression machine learning models. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2022, 422, 127800.	2.1	29
34	Free Carriers versus Self-Trapped Excitons at Different Facets of Ruddlesden-Popper Two-Dimensional Lead Halide Perovskite Single Crystals. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4965-4971.	4.6	27
35	Fe-Doping in Double Perovskite $\text{PrBaCo}_2(1-x)\text{Fe}_2x\text{O}_6$ : Insights into Structural and Electronic Effects to Enhance Oxygen Evolution Catalyst Stability. <i>Catalysts</i> , 2019, 9, 263.	3.5	25
36	Autonomous Discovery of Materials for Intercalation Electrodes. <i>Batteries and Supercaps</i> , 2020, 3, 488-498.	4.7	25

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37	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
38	Strain sensitivity of band gaps of Sn-containing semiconductors. Physical Review B, 2015, 91, .	3.2	24
39	The role of an interface in stabilizing reaction intermediates for hydrogen evolution in aprotic electrolytes. Chemical Science, 2020, 11, 3914-3922.	7.4	23
40	Band structure of MoSTe Janus nanotubes. Physical Review Materials, 2021, 5, .	2.4	23
41	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
42	Structural and chemical mechanisms governing stability of inorganic Janus nanotubes. Npj Computational Materials, 2021, 7, .	8.7	22
43	Vibrational characterization of dinaphthylpolyyenes: A model system for the study of end-capped $sp$ carbon chains. Journal of Chemical Physics, 2011, 135, 194501.	3.0	21
44	Metastability at Defective Metal Oxide Interfaces and Nanoconfined Structures. Advanced Materials Interfaces, 2020, 7, 1902090.	3.7	20
45	Determination of Conduction and Valence Band Electronic Structure of $LaTiO_{xN_y}$ Thin Film. ChemSusChem, 2017, 10, 2099-2106.	6.8	19
46	Electronic Structure and Trap States of Two-Dimensional Ruddlesden-Popper Perovskites with the Relaxed Goldschmidt Tolerance Factor. ACS Applied Electronic Materials, 2020, 2, 1402-1412.	4.3	19
47	Data Management Plans: the Importance of Data Management in the BIG-MAP Project**. Batteries and Supercaps, 2021, 4, 1803-1812.	4.7	19
48	Synergetic Surface Sensitivity of Photoelectrochemical Water Oxidation on $TiO_2$ (Anatase) Electrodes. Journal of Physical Chemistry C, 2017, 121, 6024-6032.	3.1	18
49	Workflow Engineering in Materials Design within the BATTERY 2030+ Project. Advanced Energy Materials, 2022, 12, .	19.5	18
50	Synergistic effects in oxygen evolution activity of mixed iridium-ruthenium pyrochlores. Electrochimica Acta, 2021, 366, 137327.	5.2	17
51	Towards autonomous high-throughput multiscale modelling of battery interfaces. Energy and Environmental Science, 2022, 15, 579-594.	30.8	17
52	Anisotropic Proton and Oxygen Ion Conductivity in Epitaxial $Ba_2In_2O_5$ Thin Films. Journal of Physical Chemistry C, 2017, 121, 21797-21805.	3.1	16
53	Carbon $sp$ chains in graphene nanoholes. Journal of Physics Condensed Matter, 2012, 24, 104019.	1.8	15
54	Role of the Band Gap for the Interaction Energy of Coadsorbed Fragments. Journal of Physical Chemistry C, 2017, 121, 18608-18614.	3.1	15

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55	Exploring the Intrinsic Point Defects in Cesium Copper Halides. Journal of Physical Chemistry C, 2021, 125, 1592-1598.	3.1	15
56	Theoretical Insight on Anion Ordering, Strain, and Doping Engineering of the Oxygen Evolution Reaction in BaTaO <sub>2</sub> N. Chemistry of Materials, 2021, 33, 3297-3303.	6.7	15
57	Nanotubes from Ternary WS <sub>2</sub> (1- <i>x</i> )Se <sub>2</sub> <i>x</i> Alloys: Stoichiometry Modulated Tunable Optical Properties. Journal of the American Chemical Society, 2022, 144, 10530-10542.	13.7	15
58	Tribology of the lubricant quantized sliding state. Journal of Chemical Physics, 2009, 131, 174711.	3.0	13
59	Bandgap Engineering of Double Perovskites for One- and Two-photon Water Splitting. Materials Research Society Symposia Proceedings, 2013, 1523, 601.	0.1	13
60	Band-gap engineering of functional perovskites through quantum confinement and tunneling. Physical Review B, 2015, 91, .	3.2	13
61	Defect Chemistry and Electrical Conductivity of Sm-Doped La <sub>1-x</sub> Sr <sub>x</sub> CoO <sub>3</sub> for Solid Oxide Fuel Cells. Journal of Physical Chemistry C, 2017, 121, 15017-15027.	3.1	13
62	Towards photoferroic materials by design: recent progress and perspectives. JPhys Energy, 2020, 2, 011001.	5.3	13
63	Role of transverse displacements for a quantized-velocity state of a lubricant. Journal of Physics Condensed Matter, 2008, 20, 354005.	1.8	12
64	Automatic Migration Path Exploration for Multivalent Battery Cathodes using Geometrical Descriptors. Batteries and Supercaps, 2021, 4, 1516-1524.	4.7	11
65	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
66	Effects of the cooperative interaction on the diffusion of hydrogen on MgO(100). Journal of Chemical Physics, 2018, 149, 034704.	3.0	10
67	Yttrium Tantalum Oxynitride Multiphases as Photoanodes for Water Oxidation. Journal of Physical Chemistry C, 2019, 123, 26211-26217.	3.1	9
68	Enhancing Oxygen Evolution Reaction Activity by Using Switchable Polarization in Ferroelectric InSnO <sub>2</sub> N. ACS Catalysis, 2021, 11, 12692-12700.	11.2	9
69	On the thermoelectric properties of Nb-doped SrTiO <sub>3</sub> epitaxial thin films. Physical Chemistry Chemical Physics, 2022, 24, 3741-3748.	2.8	9
70	Atomic-scale insights into electro-steric substitutional chemistry of cerium oxide. Physical Chemistry Chemical Physics, 2020, 22, 21900-21908.	2.8	6
71	Atomic-Scale Observation of Oxygen Vacancy-Induced Step Reconstruction in WO <sub>3</sub> . Journal of Physical Chemistry C, 2021, 125, 8456-8460.	3.1	6
72	Editorial to the Special Issue: How to Reinvent the Ways to Invent the Batteries of the Future – the Battery 2030+ Large-Scale Research Initiative Roadmap. Advanced Energy Materials, 2022, 12, .	19.5	6

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73	Observation of Biradical Spin Coupling through Hydrogen Bonds. Physical Review Letters, 2022, 128, .	7.8	6
74	Electromechanically active pair dynamics in a Gd-doped ceria single crystal. Physical Chemistry Chemical Physics, 2021, 23, 11233-11239.	2.8	5
75	Fundamental Atomic Insight in Electrocatalysis. , 2018, , 1-31.		4
76	Nonlinear Photoelectric Properties by Strained MoS <sub>2</sub> and SnO <sub>2</sub> Coreâ€Shell Nanotubes for Flexible Visible Light Photodetectors. Advanced Materials Technologies, 2021, 6, 2001105.	5.8	4
77	Autonomous Design of Photoferroic Ruddlesden-Popper Perovskites for Water Splitting Devices. Materials, 2022, 15, 309.	2.9	3
78	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
79	Chapter 3. Computational Screening of Light-absorbing Materials for Photoelectrochemical Water Splitting. RSC Energy and Environment Series, 2018, , 62-99.	0.5	2
80	Effect of high oxygen deficiency in nano-confined bismuth sesquioxide. JPhys Energy, 2020, 2, 024010.	5.3	1
81	Fundamental Atomic Insight in Electrocatalysis. , 2020, , 1473-1503.		1
82	Autonomous Discovery of Materials for Intercalation Electrodes. Batteries and Supercaps, 2020, 3, 473-473.	4.7	0
83	Role of Fe-Doping in Perovskite Oxides for the Oxygen Evolution Reaction. ECS Meeting Abstracts, 2018, , .	0.0	0