Pieremanuele Canepa

List of Publications by Year
in descending order

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72 papers	7,463 citations	76196 40 h-index	98622 67 g-index
90 all docs	90 docs citations	90 times ranked	8123 citing authors

#	Article	IF	Citations
1	Fundamentals of inorganic solid-state electrolytes for batteries. Nature Materials, 2019, 18, 1278-1291.	13.3	1,341
2	Odyssey of Multivalent Cathode Materials: Open Questions and Future Challenges. Chemical Reviews, 2017, 117, 4287-4341.	23.0	914
3	Materials Design Rules for Multivalent Ion Mobility in Intercalation Structures. Chemistry of Materials, 2015, 27, 6016-6021.	3.2	445
4	Spinel compounds as multivalent battery cathodes: a systematic evaluation based on ab initio calculations. Energy and Environmental Science, 2015, 8, 964-974.	15.6	430
5	Stability and Hydrolyzation of Metal Organic Frameworks with Paddle-Wheel SBUs upon Hydration. Chemistry of Materials, 2012, 24, 3153-3167.	3.2	368
6	Tuning the Gate Opening Pressure of Metalâ€“Organic Frameworks (MOFs) for the Selective Separation of Hydrocarbons. Journal of the American Chemical Society, 2012, 134, 15201-15204.	6.6	278
7	Atomic-Scale Influence of Grain Boundaries on Li-Ion Conduction in Solid Electrolytes for All-Solid-State Batteries. Journal of the American Chemical Society, 2018, 140, 362-368.	6.6	226
8	High magnesium mobility in ternary spinel chalcogenides. Nature Communications, 2017, 8, 1759.	5.8	212
9	Role of Structural H₂O in Intercalation Electrodes: The Case of Mg in Nanocrystalline Xerogel-V₂O₅. Nano Letters, 2016, 16, 2426-2431.	4.5	194
10	Water Reaction Mechanism in Metal Organic Frameworks with Coordinatively Unsaturated Metal Ions: MOF-74. Chemistry of Materials, 2014, 26, 6886-6895.	3.2	149
11	First-principles evaluation of multi-valent cation insertion into orthorhombic V₂O₅. Chemical Communications, 2015, 51, 13619-13622.	2.2	148
12	Elucidating the structure of the magnesium aluminum chloride complex electrolyte for magnesium-ion batteries. Energy and Environmental Science, 2015, 8, 3718-3730.	15.6	131
13	The Intercalation Phase Diagram of Mg in V₂O₅ from First-Principles. Chemistry of Materials, 2015, 27, 3733-3742.	3.2	130
14	Mechanism of Preferential Adsorption of SO₂ into Two Microporous Paddle Wheel Frameworks M(bdc)(ted)_{0.5}. Chemistry of Materials, 2013, 25, 4653-4662.	3.2	127
15	Evaluation of sulfur spinel compounds for multivalent battery cathode applications. Energy and Environmental Science, 2016, 9, 3201-3209.	15.6	121
16	Water Cluster Confinement and Methane Adsorption in the Hydrophobic Cavities of a Fluorinated Metalâ€“Organic Framework. Journal of the American Chemical Society, 2013, 135, 12615-12626.	6.6	114
17	Understanding the Initial Stages of Reversible Mg Deposition and Stripping in Inorganic Nonaqueous Electrolytes. Chemistry of Materials, 2015, 27, 3317-3325.	3.2	105
18	Interaction of Acid Gases SO₂ and NO₂ with Coordinatively Unsaturated Metal Organic Frameworks: M-MOF-74 (M = Zn, Mg, Ni, Co). Chemistry of Materials, 2017, 29, 4227-4235.	3.2	99

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19	Diffusion of Small Molecules in Metal Organic Framework Materials. Physical Review Letters, 2013, 110, 026102.	2.9	98
20	High-throughput screening of small-molecule adsorption in MOF. Journal of Materials Chemistry A, 2013, 1, 13597.	5.2	92
21	A chemical map of NaSICON electrode materials for sodium-ion batteries. Journal of Materials Chemistry A, 2021, 9, 281-292.	5.2	91
22	Toward Understanding the Different Influences of Grain Boundaries on Ion Transport in Sulfide and Oxide Solid Electrolytes. Chemistry of Materials, 2019, 31, 5296-5304.	3.2	89
23	<i>J-ICE</i>: a new<i>Jmol</i>interface for handling and visualizing crystallographic and electronic properties. Journal of Applied Crystallography, 2011, 44, 225-229.	1.9	88
24	Ionic Transport in Potential Coating Materials for Mg Batteries. Chemistry of Materials, 2019, 31, 8087-8099.	3.2	82
25	Particle Morphology and Lithium Segregation to Surfaces of the Li₇La₃Zr₂O₁₂ Solid Electrolyte. Chemistry of Materials, 2018, 30, 3019-3027.	3.2	80
26	Influence of Inversion on Mg Mobility and Electrochemistry in Spinels. Chemistry of Materials, 2017, 29, 7918-7930.	3.2	75
27	Designing interfaces in energy materials applications with first-principles calculations. Npj Computational Materials, 2019, 5, .	3.5	71
28	When metal organic frameworks turn into linear magnets. Physical Review B, 2013, 87, .	1.1	65
29	Understanding the nature of the passivation layer enabling reversible calcium plating. Energy and Environmental Science, 2020, 13, 3423-3431.	15.6	60
30	Under Pressure: Mechanochemical Effects on Structure and Ion Conduction in the Sodium-Ion Solid Electrolyte Na₃PS₄. Journal of the American Chemical Society, 2020, 142, 18422-18436.	6.6	58
31	Phase Behavior in Rhombohedral NaSiCON Electrolytes and Electrodes. Chemistry of Materials, 2020, 32, 7908-7920.	3.2	58
32	Role of Point Defects in Spinel Mg Chalcogenide Conductors. Chemistry of Materials, 2017, 29, 9657-9667.	3.2	56
33	An efficient algorithm for finding the minimum energy path for cation migration in ionic materials. Journal of Chemical Physics, 2016, 145, 074112.	1.2	54
34	Probing Mg Migration in Spinel Oxides. Chemistry of Materials, 2020, 32, 663-670.	3.2	53
35	Stacking Faults Assist Lithium-Ion Conduction in a Halide-Based Superionic Conductor. Journal of the American Chemical Society, 2022, 144, 5795-5811.	6.6	50
36	Devil is in the Defects: Electronic Conductivity in Solid Electrolytes. Chemistry of Materials, 2021, 33, 7484-7498.	3.2	49

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37	Metal-free perovskites for non linear optical materials. Chemical Science, 2019, 10, 8187-8194.	3.7	46
38	Evaluation of Mg Compounds as Coating Materials in Mg Batteries. Frontiers in Chemistry, 2019, 7, 24.	1.8	46
39	Elucidating the nature of grain boundary resistance in lithium lanthanum titanate. Journal of Materials Chemistry A, 2021, 9, 6487-6498.	5.2	44
40	On the Balance of Intercalation and Conversion Reactions in Battery Cathodes. Advanced Energy Materials, 2018, 8, 1800379.	10.2	43
41	Structural, elastic, thermal, and electronic responses of small-molecule-loaded metalâ€“organic framework materials. Journal of Materials Chemistry A, 2015, 3, 986-995.	5.2	42
42	Elastic and Vibrational Properties of Î±- and Î²-PbO.. Journal of Physical Chemistry C, 2012, 116, 21514-21522.	1.5	38
43	Study of van der Waals bonding and interactions in metal organic framework materials. Journal of Physics Condensed Matter, 2014, 26, 133002.	0.7	34
44	Spectroscopic characterization of van der Waals interactions in a metal organic framework with unsaturated metal centers: MOF-74â€“Mg. Journal of Physics Condensed Matter, 2012, 24, 424203.	0.7	32
45	NMR study of small molecule adsorption in MOF-74-Mg. Journal of Chemical Physics, 2013, 138, 154704.	1.2	31
46	Crystal Structure of Na₂V₂(PO₄)₃, an Intriguing Phase Spotted in the Na₃V₂(PO₄)₃â€“Na₁V₂(PO₄)<sub>3</sub System. Chemistry of Materials, 2022, 34, 451-462.	3.2	31
47	Favorable Interfacial Chemomechanics Enables Stable Cycling of High-Li-Content Liâ€“In/Sn Anodes in Sulfide Electrolyte-Based Solid-State Batteries. Chemistry of Materials, 2021, 33, 6029-6040.	3.2	28
48	Affinity of hydroxyapatite (001) and (010) surfaces to formic and alendronic acids: a quantum-mechanical and infrared study. Physical Chemistry Chemical Physics, 2011, 13, 1099-1111.	1.3	27
49	Phase stability and sodium-vacancy orderings in a NaSICON electrode. Journal of Materials Chemistry A, 2021, 10, 209-217.	5.2	24
50	Comparison of a calculated and measured XANES spectrum of Î±-Fe2O3. Physical Chemistry Chemical Physics, 2011, 13, 12826.	1.3	23
51	Insights into the Rich Polymorphism of the Na⁺ Ion Conductor Na₃PS₄ from the Perspective of Variable-Temperature Diffraction and Spectroscopy. Chemistry of Materials, 2021, 33, 5652-5667.	3.2	23
52	Magnesium ion mobility in post-spinels accessible at ambient pressure. Chemical Communications, 2017, 53, 5171-5174.	2.2	21
53	Towards autonomous high-throughput multiscale modelling of battery interfaces. Energy and Environmental Science, 2022, 15, 579-594.	15.6	17
54	Rational Design of Mixed Polyanion Electrodes Na_{<i>x</i>}V₂P_{3â€“<i>i</i>}(Si/S)_{<i>i</i>}O₁₂ for Sodium Batteries. Chemistry of Materials, 2022, 34, 3373-3382.	3.2	16

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55	The resistive nature of decomposing interfaces of solid electrolytes with alkali metal electrodes. Journal of Materials Chemistry A, 2022, 10, 19732-19742.	5.2	14
56	Design and Characterization of Host Frameworks for Facile Magnesium Transport. Annual Review of Materials Research, 2022, 52, 129-158.	4.3	11
57	Understanding the Structural and Electronic Properties of Bismuth Trihalides and Related Compounds. Inorganic Chemistry, 2020, 59, 3377-3386.	1.9	9
58	Superionic Conduction in the Plastic Crystal Polymorph of Na₄P₂S₆. ACS Energy Letters, 2022, 7, 1403-1411.	8.8	9
59	Computational analysis and identification of battery materials. Physical Sciences Reviews, 2019, 4, .	0.8	8
60	Searching Ternary Oxides and Chalcogenides as Positive Electrodes for Calcium Batteries. Chemistry of Materials, 2021, 33, 5809-5821.	3.2	8
61	Unlocking the origin of compositional fluctuations in InGaN light emitting diodes. Physical Review Materials, 2021, 5, .	0.9	7
62	H₂O and CO₂ surface contamination of the lithium garnet Li₇La₃Zr₂O₁₂ solid electrolyte. Journal of Materials Chemistry A, 2022, 10, 4960-4973.	5.2	6
63	Assessing the formation of weak sodium complexes with negatively charged ligands. Physical Chemistry Chemical Physics, 2016, 18, 13118-13125.	1.3	4
64	Solid Electrolytes in the Spotlight. Chemistry of Materials, 2022, 34, 463-467.	3.2	4
65	CHAPTER 4. Theoretical Modelling of Multivalent Ions in Inorganic Hosts. RSC Energy and Environment Series, 2019, , 79-113.	0.2	2
66	Continuum Model of Gas Uptake for Inhomogeneous Fluids. Journal of Physical Chemistry C, 2017, 121, 17625-17632.	1.5	0
67	4. Battery Materials. , 2018, , 75-260.		0
68	(Invited) Revisiting the Structureâ€“Property Relationships in NaSICON Electrode and Electrolytes. ECS Meeting Abstracts, 2021, MA2021-01, 456-456.	0.0	0
69	Phase Behavior in Nasicon Electrolytes and Electrodes. ECS Meeting Abstracts, 2020, MA2020-02, 1002-1002.	0.0	0
70	Electrochemical Stability and Ionic Transport in Coating Materials for Mg Batteries. ECS Meeting Abstracts, 2020, MA2020-02, 212-212.	0.0	0
71	A Chemical Map of Nasicon Electrode Materials for Sodium-Ion Batteries. ECS Meeting Abstracts, 2021, MA2021-02, 214-214.	0.0	0
72	(Invited) Crystal Chemistry of NaxMM'(PO4)3 Nasicon Electrodes (M,M' = V, Fe, Mn, Ti, Cr). ECS Meeting Abstracts, 2021, MA2021-02, 211-211.	0.0	0