Mathieu SaubanÃ¨re

List of Publications by Year
in descending order

44 papers	4,341 citations	331670 21 h-index	254184 43 g-index
48 all docs	48 docs citations	48 times ranked	4461 citing authors

#	Article	IF	Citations
1	Local Potential Functional Embedding Theory: A Self-Consistent Flavor of Density Functional Theory for Lattices without Density Functionals. Computation, 2022, 10, 45.	2.0	6
2	Influence of local structural distortion on the magnetism of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Na</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math> compounds. Physical Review B, 2022, 105, .	3.2	4
3	Structure, Magnetism, and First-Principles Modeling of the Na_{0.5}La_{0.5}RuO₃ Perovskite. Chemistry of Materials, 2021, 33, 600-607.	6.7	5
4	Householder-transformed density matrix functional embedding theory. Physical Review B, 2021, 104, .	3.2	9
5	The Structural Stability of P2-Layered Na-Based Electrodes during Anionic Redox. Joule, 2020, 4, 420-434.	24.0	89
6	Alkali-Glass Behavior in Honeycomb-Type Layered Li_{3â€“x}Na_xNi₂SbO₆ Solid Solution. Inorganic Chemistry, 2019, 58, 11546-11552.	4.0	15
7	Site-occupation Green's function embedding theory: A density functional approach to dynamical impurity solvers. Physical Review B, 2019, 100, .	3.2	4
8	Charge Transfer Band Gap as an Indicator of Hysteresis in Li-Disordered Rock Salt Cathodes for Li-Ion Batteries. Journal of the American Chemical Society, 2019, 141, 11452-11464.	13.7	81
9	Unified picture of anionic redox in Li/Na-ion batteries. Nature Materials, 2019, 18, 496-502.	27.5	335
10	Synthesis and Electrochemical Activity of Some Na(Li)â€Rich Ruthenium Oxides with the Feasibility to Stabilize Ru⁶⁺. Advanced Energy Materials, 2019, 9, 1803674.	19.5	28
11	Electrostatic Interactions versus Second Order Jahnâ€“Teller Distortion as the Source of Structural Diversity in Li₃MO₄ Compounds (M = Ru, Nb, Sb and Ta). Chemistry of Materials, 2018, 30, 392-402.	6.7	15
12	Modelling CO2 transfer in foil ripened semi-hard Swiss-type cheese. Journal of Food Engineering, 2018, 222, 73-83.	5.2	1
13	Atomic Structure of 2 nm Size Metallic Cobalt Prepared by Electrochemical Conversion: An in Situ Pair Distribution Function Study. Journal of Physical Chemistry C, 2018, 122, 23861-23866.	3.1	14
14	Anionic Redox Activity in a Newly Znâ€Doped Sodium Layered Oxide P2â€Na_{2/3}Mn_{1â^'}_yZn_yO₂ (0 <) TjET Qq0 0 0 rgBT /Ov	19.5	182
15	Competition between Metal Dissolution and Gas Release in Li-Rich Li₃Ru_yIr_{1â€“y}O₄ Model Compounds Showing Anionic Redox. Chemistry of Materials, 2018, 30, 7682-7690.	6.7	25
16	Chemical Activity of the Peroxide/Oxide Redox Couple: Case Study of Ba₅Ru₂O₁₁ in Aqueous and Organic Solvents. Chemistry of Materials, 2018, 30, 3882-3893.	6.7	8
17	(Invited) The Paradox of High-Energy Density Materials for Li-Ion Batteries. ECS Meeting Abstracts, 2018, , .	0.0	0
18	Evidence for anionic redox activity in a tridimensional-ordered Li-rich positive electrodeÂÎ²-Li2IrO3. Nature Materials, 2017, 16, 580-586.	27.5	290

#	Article	IF	Citations
19	Requirements for reversible extra-capacity in Li-rich layered oxides for Li-ion batteries. Energy and Environmental Science, 2017, 10, 266-274.	30.8	269
20	Activation of surface oxygen sites on an iridium-based model catalyst for the oxygen evolution reaction. Nature Energy, 2017, 2, .	39.5	435
21	Approaching the limits of cationic and anionic electrochemical activity with the Li-rich layered rocksalt Li3IrO4. Nature Energy, 2017, 2, 954-962.	39.5	138
22	Requirements for Reversible Extra-Capacity in Li-Rich Layered Oxides for Li-Ionbatteries. ECS Meeting Abstracts, 2017, , .	0.0	0
23	Interaction-energy functional of the Hubbard model: Local formulation and application to low-dimensional lattices. Physical Review B, 2016, 94, .	3.2	7
24	Electrochemical activity and high ionic conductivity of lithium copper pyroborate Li₆CuB₄O₁₀. Physical Chemistry Chemical Physics, 2016, 18, 14960-14969.	2.8	14
25	A₂VO(SO₄)₂ (A = Li, Na) as Electrodes for Li-Ion and Na-Ion Batteries. Chemistry of Materials, 2016, 28, 6637-6643.	6.7	22
26	Strong Oxygen Participation in the Redox Governing the Structural and Electrochemical Properties of Na-Rich Layered Oxide Na₂IrO₃. Chemistry of Materials, 2016, 28, 8278-8288.	6.7	132
27	An appraisal of the impact of compositional and ripening parameters on CO2 diffusivity in semi-hard cheese. Food Chemistry, 2016, 194, 1172-1179.	8.2	7
28	A Fully Ordered Triplite, LiCuSO₄F. Chemistry of Materials, 2016, 28, 1607-1610.	6.7	9
29	The intriguing question of anionic redox in high-energy density cathodes for Li-ion batteries. Energy and Environmental Science, 2016, 9, 984-991.	30.8	453
30	Atomistic Modeling of Electrode Materials for Li-Ion Batteries: From Bulk to Interfaces. Green Energy and Technology, 2016, , 1-36.	0.6	2
31	Visualization of O-O peroxo-like dimers in high-capacity layered oxides for Li-ion batteries. Science, 2015, 350, 1516-1521.	12.6	659
32	Influence of polymorphism on the electrochemical behavior of M Sb negative electrodes in Li/Na batteries. Journal of Power Sources, 2015, 280, 695-702.	7.8	21
33	Unraveling the Structure of Iron(III) Oxalate Tetrahydrate and Its Reversible Li Insertion Capability. Chemistry of Materials, 2015, 27, 1631-1639.	6.7	30
34	Reversible Li-Intercalation through Oxygen Reactivity in Li-Rich Li-Fe-Te Oxide Materials. Journal of the Electrochemical Society, 2015, 162, A1341-A1351.	2.9	47
35	Li2Cu2O(SO4)2: a Possible Electrode for Sustainable Li-Based Batteries Showing a 4.7 V Redox Activity vs Li+/Li0. Chemistry of Materials, 2015, 27, 3077-3087.	6.7	31
36	Origin of voltage decay in high-capacity layered oxide electrodes. Nature Materials, 2015, 14, 230-238.	27.5	757

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37	An intuitive and efficient method for cell voltage prediction of lithium and sodium-ion batteries. Nature Communications, 2014, 5, 5559.	12.8	39
38	Density-matrix functional theory of strongly correlated fermions on lattice models and minimal-basis Hamiltonians. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	8
39	Lattice density-functional theory of the attractive Hubbard model. Physical Review B, 2014, 90, .	3.2	8
40	Origin of the Voltage Hysteresis in the CoP Conversion Material for Li-Ion Batteries. Journal of Physical Chemistry C, 2013, 117, 837-849.	3.1	87
41	Density-matrix functional study of the Hubbard model on one- and two-dimensional bipartite lattices. Physical Review B, 2011, 84, .	3.2	18
42	First principles theoretical study of complex magnetic order in transitionâ€metal nanowires. Physica Status Solidi (B): Basic Research, 2010, 247, 2610-2620.	1.5	13
43	Electronic and magnetic properties of Co and Ni impurities in Cu wires: First-principles investigation of local moment formation in one dimension. Physical Review B, 2010, 82, .	3.2	3
44	Scaling and transferability of the interaction-energy functional of the inhomogeneous Hubbard model. Physical Review B, 2009, 79, .	3.2	17