Marie-Liesse Doublet

List of Publications by Year in descending order

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114 papers 9,440 citations

70961 41 h-index 96 g-index

122 all docs $\begin{array}{c} 122 \\ \text{docs citations} \end{array}$

times ranked

122

8708 citing authors

#	Article	IF	CITATIONS
1	Reversible anionic redox chemistry in high-capacity layered-oxide electrodes. Nature Materials, 2013, 12, 827-835.	13.3	1,192
2	Origin of voltage decay in high-capacity layered oxide electrodes. Nature Materials, 2015, 14, 230-238.	13.3	757
3	Visualization of O-O peroxo-like dimers in high-capacity layered oxides for Li-ion batteries. Science, 2015, 350, 1516-1521.	6.0	659
4	Mixed-Valence Li/Fe-Based Metal–Organic Frameworks with Both Reversible Redox and Sorption Properties. Angewandte Chemie - International Edition, 2007, 46, 3259-3263.	7.2	583
5	The intriguing question of anionic redox in high-energy density cathodes for Li-ion batteries. Energy and Environmental Science, 2016, 9, 984-991.	15.6	453
6	Activation of surface oxygen sites on an iridium-based model catalyst for the oxygen evolution reaction. Nature Energy, $2017, 2, .$	19.8	435
7	High Performance Li ₂ Ru _{1–<i>y</i>} Mn _{<i>y</i>} O ₃ (0.2 â‰) Chemistry of Materials, 2013, 25, 1121-1131.	¤Tj ETQq1 3.2	1 0.78431 365
8	Unified picture of anionic redox in Li/Na-ion batteries. Nature Materials, 2019, 18, 496-502.	13.3	335
9	A 3.90 V iron-based fluorosulphate material for lithium-ion batteries crystallizing in the triplite structure. Nature Materials, 2011, 10, 772-779.	13.3	301
10	Evidence for anionic redox activity in a tridimensional-ordered Li-rich positive electrode \hat{Al}^2 -Li2IrO3. Nature Materials, 2017, 16, 580-586.	13.3	290
11	Requirements for reversible extra-capacity in Li-rich layered oxides for Li-ion batteries. Energy and Environmental Science, 2017, 10, 266-274.	15.6	269
12	Electrochemical Reactivity and Design of NiP2 Negative Electrodes for Secondary Li-lon Batteries. Chemistry of Materials, 2005, 17, 6327-6337.	3.2	229
13	FeP:  Another Attractive Anode for the Li-Ion Battery Enlisting a Reversible Two-Step Insertion/Conversion Process. Chemistry of Materials, 2006, 18, 3531-3538.	3.2	181
14	Unlocking anionic redox activity in O3-type sodium 3d layered oxides via Li substitution. Nature Materials, 2021, 20, 353-361.	13.3	155
15	Approaching the limits of cationic and anionic electrochemical activity with the Li-rich layered rocksalt Li3IrO4. Nature Energy, 2017, 2, 954-962.	19.8	138
16	Strong Oxygen Participation in the Redox Governing the Structural and Electrochemical Properties of Na-Rich Layered Oxide Na ₂ IrO ₃ . Chemistry of Materials, 2016, 28, 8278-8288.	3.2	132
17	A Chemical Approach to Raise Cell Voltage and Suppress Phase Transition in O3 Sodium Layered Oxide Electrodes. Advanced Energy Materials, 2018, 8, 1702599.	10.2	127
18	Electrical Conductivity and Spin Crossover:  A New Achievement with a Metal Bis Dithiolene Complex. Inorganic Chemistry, 2007, 46, 8548-8559.	1.9	104

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19	Thermodynamic origin of dendrite growth in metal anode batteries. Energy and Environmental Science, 2020, 13, 5186-5197.	15.6	101
20	Updated references for the structural, electronic, and vibrational properties of TiO2(B) bulk using first-principles density functional theory calculations. Journal of Chemical Physics, 2009, 130, 204501.	1.2	99
21	Li4NiTeO6 as a positive electrode for Li-ion batteries. Chemical Communications, 2013, 49, 11376.	2.2	96
22	The Structural Stability of P2-Layered Na-Based Electrodes during Anionic Redox. Joule, 2020, 4, 420-434.	11.7	89
23	Origin of the Voltage Hysteresis in the CoP Conversion Material for Li-lon Batteries. Journal of Physical Chemistry C, 2013, 117, 837-849.	1.5	87
24	Design of Electrode Materials for Lithium-Ion Batteries: The Example of Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2010, 114, 9518-9527.	1.5	82
25	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.	6.6	81
26	Correlating ligand-to-metal charge transfer with voltage hysteresis in a Li-rich rock-salt compound exhibiting anionic redox. Nature Chemistry, 2021, 13, 1070-1080.	6.6	75
27	P-Redox Mechanism at the Origin of the High Lithium Storage in NiP2-Based Batteries. Chemistry of Materials, 2009, 21, 298-308.	3.2	71
28	Electrolyte Reactivity in the Double Layer in Mg Batteries: An Interface Potential-Dependent DFT Study. Journal of the American Chemical Society, 2020, 142, 5146-5153.	6.6	71
29	Interface electrochemistry in conversion materials for Li-ion batteries. Journal of Materials Chemistry, 2011, 21, 10134.	6.7	66
30	Redox-Induced Structural Change in Anode Materials Based on Tetrahedral (MPn4)x-Transition Metal Pnictides. Chemistry of Materials, 2004, 16, 1002-1013.	3.2	63
31	The Mechanism of Acetylene Cyclotrimerization Catalyzed by the fac-lrP3+ Fragment: The Relationship between Fluxionality and Catalysis. Organometallics, 1994, 13, 2010-2023.	1.1	62
32	The LixVPn4 Ternary Phases (Pn = P, As):  Rigid Networks for Lithium Intercalation/Deintercalation. Chemistry of Materials, 2002, 14, 4126-4133.	3.2	61
33	Origin of the 3.6 V to 3.9 V voltage increase in the LiFeSO4F cathodes for Li-ion batteries. Energy and Environmental Science, 2012, 5, 9584.	15.6	58
34	Electrochemical Behaviors of Binary and Ternary Manganese Phosphides. Chemistry of Materials, 2005, 17, 5817-5823.	3.2	57
35	An ab initio study of surface electrochemical disproportionation: The case of a water monolayer adsorbed on a $Pd(111)$ surface. Catalysis Today, 2013, 202, 87-97.	2,2	55
36	Fell/Felll mixed-valence state induced by Li-insertion into the metal-organic-framework Mil53(Fe): A DFT+U study. Journal of Power Sources, 2011, 196, 3426-3432.	4.0	51

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37	The LixMPn4 phases (M/Pn = Ti/P, V/As): new negative electrode materials for lithium ion rechargeable batteries. Electrochimica Acta, 2004, 49, 2325-2332.	2.6	49
38	Redox mechanism in the binary transition metal phosphide Cu3P. Journal of Physics and Chemistry of Solids, 2006, 67, 1252-1257.	1.9	47
39	Direct Correlation between the ³¹ P MAS NMR Response and the Electronic Structure of Some Transition Metal Phosphides. Journal of Physical Chemistry C, 2008, 112, 20481-20490.	1.5	47
40	Reversible Li-Intercalation through Oxygen Reactivity in Li-Rich Li-Fe-Te Oxide Materials. Journal of the Electrochemical Society, 2015, 162, A1341-A1351.	1.3	47
41	Synthesis, Crystal Structure, Electrical Properties and Electronic Band Structure of (NHyMe4-y)x[M(dmit)2] Complexes (M = Ni, Pd, Pt; dmit2- = 2-Thioxo-1,3-dithiole-4,5-dithiolato). Inorganic Chemistry, 1994, 33, 3401-3414.	1.9	42
42	Zn _{0.35} Co _{0.65} O – A Stable and Highly Active Oxygen Evolution Catalyst Formed by Zinc Leaching and Tetrahedral Coordinated Cobalt in Wurtzite Structure. Advanced Energy Materials, 2019, 9, 1900328.	10.2	41
43	The Ir–OOOO–Ir transition state and the mechanism of the oxygen evolution reaction on IrO ₂ (110). Energy and Environmental Science, 2022, 15, 2519-2528.	15.6	40
44	An intuitive and efficient method for cell voltage prediction of lithium and sodium-ion batteries. Nature Communications, 2014, 5, 5559.	5.8	39
45	Phase Diagrams for Systems with Low Free Energy Variation:  A Coupled Theory/Experiments Method Applied to Li-Graphite. Journal of Physical Chemistry C, 2008, 112, 3982-3988.	1.5	37
46	Origin of the Voltage Hysteresis of MgH ₂ Electrodes in Lithium Batteries. Journal of Physical Chemistry C, 2015, 119, 17044-17052.	1.5	37
47	Single-Step Synthesis of FeSO ₄ F _{1–<i>y</i>} OH _{<i>y</i>} (0 ≤i>y)	Тį <mark>ЕТ</mark> Qq1	1 ₃₅ 784314
48	Leading interactions in thel²â°'SrV6O15compound. Physical Review B, 2005, 71, .	1.1	34
49	Structural, magnetic and redox properties of a new cathode material for Li-ion batteries: the iron-based metal organic framework. Ionics, 2008, 14, 279-283.	1.2	34
50	On the Reactivity of Li8-yMnyP4 toward Lithium. Chemistry of Materials, 2005, 17, 3627-3635.	3.2	33
51	Reversible Sodium and Lithium Insertion in Iron Fluoride Perovskites. Advanced Functional Materials, 2018, 28, 1802057.	7.8	33
52	Interplay between Magnetic and Orbital Ordering in the Strongly Correlated Cobalt Oxide: A DFT + <i>U</i> Study. Journal of Physical Chemistry C, 2010, 114, 21750-21756.	1.5	32
53	Conceptual Surface Electrochemistry and New Redox Descriptors. Journal of Physical Chemistry C, 2014, 118, 19023-19031.	1.5	31
54	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.	3.2	31

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55	Electronic Structure of the \$mathsf{alpha}\$-(BEDT-TTF)\$mathsf{_2}\$MHg(XCN)\$mathsf{_4}\$ (M = Tl,) Organic Metal \$alpha\$-(BEDT-TTF)\$mathsf{_2}\$TlHg(Se\$mathsf{_{m 1-x}}\$S\$mathsf{_{m 1-x}}\$S\$mathsf{_m 1-x}\$S\$mathsf{_{m 1-x}}\$S\$mathsf{_{m 1		
56	Electrochemical Mg alloying properties along the Sb1-xBix solid solution. Electrochimica Acta, 2018, 259, 276-283.	2.6	30
57	Density functional theory analysis of the local chemical bonds in the periodic tantalum dichalcogenides TaX2 (X=S, Se, Te). Journal of Chemical Physics, 2000, 113, 5879-5890.	1.2	29
58	A New Family of Molecular Metals Based on Bis(ethylenethio)tetrathiafulvalene (BET-TTF) and Octahedral Counterions. Chemistry of Materials, 1995, 7, 1558-1567.	3.2	28
59	Activation of anionic redox in d0 transition metal chalcogenides by anion doping. Nature Communications, 2021, 12, 5485.	5.8	26
60	Factors affecting the metallic versus semiconducting properties of charge transfer salts containing [M(dddt)2]2 and [M(dmit)2]2 (M = Pd, Pt) dimers. Solid State Communications, 1993, 88, 699-703.	0.9	25
61	Anion Conformation and Physical Properties in BETS Salts with the Nitroprusside Anion and its Related Ruthenium Halide (X = Cl, Br) Mononitrosyl Complexes: \hat{l}_{r} -(BETS)4[Fe(CN)5NO], (BETS)2[RuBr5NO], and (BETS)2[RuCl5NO]. European Journal of Inorganic Chemistry, 2001, 2001, 2797.	1.0	25
62	Competition between Metal Dissolution and Gas Release in Li-Rich Li ₃ Ru _{<i>y</i>} Ir _{1â€"<i>y</i>} O ₄ Model Compounds Showing Anionic Redox. Chemistry of Materials, 2018, 30, 7682-7690.	3.2	25
63	Concerning the first-order transition in the ?-phase (BEDT-TTF)4PtCl6 . C6H5CN. Journal De Physique, I, 1994, 4, 1479-1490.	1.2	24
64	New Insights on the Reversible Lithiation Mechanism of $TiO \leq 2 \leq s$ by Operando X-ray Absorption Spectroscopy and X-ray Diffraction Assisted by First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 27210-27218.	1.5	23
65	A $<$ sub $>$ 2 $<$ /sub $>$ VO(SO $<$ sub $>$ 4 $<$ /sub $>$) $<$ sub $>$ 2 $<$ /sub $>$ (A = Li, Na) as Electrodes for Li-lon and Na-lon Batteries. Chemistry of Materials, 2016, 28, 6637-6643.	3.2	22
66	Influence of polymorphism on the electrochemical behavior of M Sb negative electrodes in Li/Na batteries. Journal of Power Sources, 2015, 280, 695-702.	4.0	21
67	The Electrochemical Sodiation of Sb Investigated by Operando X-ray Absorption and 121Sb M¶ssbauer Spectroscopy: What Does One Really Learn?. Batteries, 2018, 4, 25.	2.1	20
68	Unexpected band gap increase in the Fe2VAl Heusler compound. Materials Today Physics, 2020, 13, 100203.	2.9	20
69	Progress in the lithium insertion mechanism in Cu3P. Ionics, 2005, 11, 36-45.	1.2	19
70	Determination of Lithium Insertion Sites in LixTiP4(x= 2â^'11) by Electron Energy-Loss Spectroscopy. Journal of Physical Chemistry C, 2007, 111, 3996-4002.	1.5	19
71	Palladiumâ€"Silver Mesowires for the Extended Detection of H ₂ . ACS Applied Materials & amp; Interfaces, 2013, 5, 310-318.	4.0	18
72	Structure-Property Correlations in the Platinum Oxide and Palladium Sulfide Bronzes with Columnar Chains of Square-Planar TX4 Units ($T = Pt$, $X = O$; $T = Pd$, $X = S$). Journal of the American Chemical Society, 1994, 116, 2115-2120.	6.6	17

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73	Metallic conductivity in a disordered charge-transfer salt derived from cis-BET-TTF. Synthetic Metals, 1997, 86, 2145-2146.	2.1	16
74	An Oxysulfate Fe2O(SO4)2 Electrode for Sustainable Li-Based Batteries. Journal of the American Chemical Society, 2014, 136, 12658-12666.	6.6	16
75	Unveiling Pseudocapacitive Charge Storage Behavior in FeWO ₄ Electrode Material by Operando Xâ€Ray Absorption Spectroscopy. Small, 2020, 16, e2002855.	5.2	16
76	The electrochemical activity of the nitrosyl ligand in copper nitroprusside: a new possible redox mechanism for lithium battery electrode materials?. Electrochimica Acta, 2017, 257, 364-371.	2.6	15
77	Electrostatic Interactions versus Second Order Jahn–Teller Distortion as the Source of Structural Diversity in Li ₃ MO ₄ Compounds (M = Ru, Nb, Sb and Ta). Chemistry of Materials, 2018, 30, 392-402.	3.2	15
78	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.	1.5	14
79	H2O photodissociation dynamics based on potential energy surfaces from density functional calculations. Journal of Chemical Physics, 1995, 103, 2538-2547.	1.2	13
80	Elucidation of Active Oxygen Sites upon Delithiation of Li ₃ IrO ₄ . ACS Energy Letters, 2021, 6, 140-147.	8.8	12
81	Structural and electronic properties of the molecular conductors (EDTTTF)x[Pd(dmit)2]y(x:y=2:3 and) Tj ETQq1	1 0,7,8431	.4 rgBT /Over
82	A new theoretical approach for the electrical properties of TiX2 (X=S, Se, Te) phases with density functional calculations. Journal of Chemical Physics, 1998, 108, 649-658.	1.2	11
83	Lithium insertion/deinsertion mechanisms in the transition metal pnictides LixMPn4. Ionics, 2003, 9, 56-63.	1.2	9
84	A Fully Ordered Triplite, LiCuSO ₄ F. Chemistry of Materials, 2016, 28, 1607-1610.	3.2	9
85	Stacking Versatility in Alkali-Mixed Honeycomb Layered NaKNi ₂ TeO ₆ . Inorganic Chemistry, 2021, 60, 14310-14317.	1.9	9
86	Advancement of the Homogeneous Background Method for the Computational Simulation of Electrochemical Interfaces. Journal of Chemical Theory and Computation, 2022, 18, 1883-1893.	2.3	9
87	Comparison of the electronic structures of isostructural (BEDT-TTF)3(HSO4)2 and [Ni(dddt)2] 3(HSO4)2 molecular metals. Journal De Physique, I, 1994, 4, 1439-1450.	1.2	8
88	Synthesis, electrical behaviour, and crystal and electronic band structures of two different phases of the (SMeEt2)[Pd(dmit)2]2 salt. Consequences of cationic disorder on the electrical properties. Journal of Materials Chemistry, 2001, 11, 2205-2210.	6.7	8
89	Redox mechanism in the NiP2 electrode for Li-ion batteries: A DFT study coupled with local chemical bond analyses. Ionics, 2008, 14, 197-202.	1.2	8
90	Chemical Activity of the Peroxide/Oxide Redox Couple: Case Study of Ba ₅ Ru ₂ O ₁₁ in Aqueous and Organic Solvents. Chemistry of Materials, 2018, 30, 3882-3893.	3.2	8

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91	New p-type Al-substituted SrSnO ₃ perovskites for TCO applications?. Chemical Communications, 2020, 56, 2566-2569.	2.2	7
92	Investigation of alkali and alkaline earth solvation structures in tetraglyme solvent. Physical Chemistry Chemical Physics, 2021, 23, 26120-26129.	1.3	7
93	Inhibited superconductivity induced by localization effects in (EDT-TTF)2[Pd(dmit)2]2. Synthetic Metals, 1993, 56, 2833-2838.	2.1	6
94	Correlation and dimerization effects on the physical behavior of the NR4[Ni(dmit)2]2 charge transfer salts: A density matrix renormalization group study of the quarter-filling t–J model. Journal of Chemical Physics, 1999, 110, 1767-1773.	1.2	6
95	Electronic properties of isostructural organic conductors (ET)3(HSO4)2 and [Ni(dddt)2]3(HSO4)2. Thermopower and tight-binding calculations. Synthetic Metals, 1995, 71, 1867-1868.	2.1	5
96	Comparison of the electronic structures of the BEDT-TTF4[$M(CN)4$] ($M = Ni, Pt$) and BEDT-TTF4[$M(C2O4)2$] ($M = Pt, Cu$) salts. Structural requirements for hidden Fermi surface nesting. Journal De Physique, I, 1993, 3, 2451-2461.	1.2	5
97	Interplay between structural, magnetic properties and calculated band structures of (EDT-TTF)2[M(dmit)2]2 where $M = Ni$, Pd . Synthetic Metals, 1995, 70, 1063-1064.	2.1	4
98	Magnetoresistance in pulsed fields, band structure calculations and charge-density wave instability in (TSeT)2Cl. Synthetic Metals, 1995, 70, 1279-1280.	2.1	4
99	Why has 1T-TaTe2 not yet been synthetized? A DFT contribution Synthetic Metals, 1999, 103, 2679-2682.	2.1	3
100	Crystal structure, band structure and electrical properties of \hat{l}^2 -(BEDT-TTF)2SbF6 grown on a Si(001) electrode. Synthetic Metals, 2010, 160, 556-560.	2.1	3
101	Access to Ru(IV)–Ru(V) and Ru(V)–Ru(VI) Redox in Layered Li ₇ RuO ₆ via Intercalation Reactions. Chemistry of Materials, 2022, 34, 3724-3735.	3.2	3
102	Effect of the cooling rate on the transverse magnetoresistance of (TSeT)2Cl in its charge-density wave ground state. Physica B: Condensed Matter, 1995, 211, 286-289.	1.3	2
103	Similarities between the t-J and Hubbard models in weakly correlated regimes. European Physical Journal B, 2002, 28, 49-54.	0.6	2
104	Atomistic Modeling of Electrode Materials for Li-Ion Batteries: From Bulk to Interfaces. Green Energy and Technology, 2016, , 1-36.	0.4	2
105	Structure and properties of BETS salts: \hat{l}^2 -(BETS)8(Cu2Cl6)(CuCl4), \hat{l}_1 -(BETS)2(CuCl2) and (BETS)2(CuCl4). Comptes Rendus De L'Academie Des Sciences - Series IIc: Chemistry, 2001, 4, 149-160.	0.1	1
106	New salts derived from organic donor molecules with long-living excited states counter-ions. Synthetic Metals, 2003, 133-134, 377-380.	2.1	1
107	(BETS)2[RuX5NO] (X=Cl, Br): an explanation of different conductive properties through structural and spectroscopic studies. Journal of Low Temperature Physics, 2006, 142, 445-448.	0.6	1
108	Chemical Design of IrS ₂ Polymorphs to Understand the Charge/Discharge Asymmetry in Anionic Redox Systems. Chemistry of Materials, 2022, 34, 325-336.	3.2	1

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109	Quantitative on-site repulsion U for the Ni(dmit)2 molecule: A DMRG study of the NR4[Ni(dmit)2]2 salts. Synthetic Metals, 1999, 103, 2062-2063.	2.1	O
110	The LixVPn4Ternary Phases (Pn: P, As): Rigid Networks for Lithium Intercalation/Deintercalation ChemInform, 2003, 34, no-no.	0.1	0
111	Redox-Induced Structural Change in Anode Materials Based on Tetrahedral (MPn4)x- Transition Metal Pnictides ChemInform, 2004, 35, no.	0.1	0
112	On the Reactivity of Li8-yMnyP4 Toward Lithium ChemInform, 2005, 36, no.	0.1	0
113	(BETS)2[RuX5NO] (X = Cl, Br): An Explanation of Different Conductive Properties Through Structural and Spectroscopic Studies. Journal of Low Temperature Physics, 2006, 142, 449-452.	0.6	0
114	Electrochemical Behaviors of Binary and Ternary Manganese Phosphides ChemInform, 2006, 37, no.	0.1	O