Marie-Liesse Doublet

List of Publications by Year in Descending Order

110 papers	7,364 citations	37 h-index	85 g-index
122 ext. papers	8,393 ext. citations	11.1 avg, IF	6.01 L-index

#	Paper	IF	Citations
110	Advancement of the Homogeneous Background Method for the Computational Simulation of Electrochemical Interfaces.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	1
109	Chemical Design of IrS2 Polymorphs to Understand the Charge/Discharge Asymmetry in Anionic Redox Systems. *Chemistry of Materials*, **2022**, 34, 325-336	9.6	
108	Elucidation of Active Oxygen Sites upon Delithiation of Li3IrO4. *ACS Energy Letters*, **2021**, 6, 140-147	20.1	5
107	Unlocking anionic redox activity in O3-type sodium 3d layered oxides via Li substitution. *Nature Materials*, **2021**, 20, 353-361	27	47
106	Investigation of alkali and alkaline earth solvation structures in tetraglyme solvent. *Physical Chemistry Chemical Physics*, **2021**, 23, 26120-26129	3.6	1
105	Activation of anionic redox in d transition metal chalcogenides by anion doping. *Nature Communications*, **2021**, 12, 5485	17.4	7
104	Stacking Versatility in Alkali-Mixed Honeycomb Layered NaKNiTeO. *Inorganic Chemistry*, **2021**, 60, 14310-14317	5.1	0
103	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	17.6	15
102	Unexpected band gap increase in the Fe2VAl Heusler compound. *Materials Today Physics*, **2020**, 13, 100283	8	10
101	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	16.4	33
100	New p-type Al-substituted SrSnO perovskites for TCO applications?. *Chemical Communications*, **2020**, 56, 2566-2569	5.8	4
99	The Structural Stability of P2-Layered Na-Based Electrodes during Anionic Redox. *Joule*, **2020**, 4, 420-434	27.8	47
98	Unveiling Pseudocapacitive Charge Storage Behavior in FeWO Electrode Material by Operando X-Ray Absorption Spectroscopy. *Small*, **2020**, 16, e2002855	11	10
97	Thermodynamic origin of dendrite growth in metal anode batteries. *Energy and Environmental Science*, **2020**, 13, 5186-5197	35.4	35
96	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	16.4	51
95	Unified picture of anionic redox in Li/Na-ion batteries. *Nature Materials*, **2019**, 18, 496-502	27	206
94	Zn0.35Co0.65O □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	21.8	27

93	A Chemical Approach to Raise Cell Voltage and Suppress Phase Transition in O3 Sodium Layered Oxide Electrodes. *Advanced Energy Materials*, **2018**, 8, 1702599	21.8	77
92	Electrochemical Mg alloying properties along the Sb1-xBix solid solution. *Electrochimica Acta*, **2018**, 259, 276-283	6.7	19
91	The Electrochemical Sodiation of Sb Investigated by Operando X-ray Absorption and 121Sb Mössbauer Spectroscopy: What Does One Really Learn?. *Batteries*, **2018**, 4, 25	5.7	18
90	Electrostatic Interactions versus Second Order Jahn–Teller Distortion as the Source of Structural Diversity in Li3MO4 Compounds (M = Ru, Nb, Sb and Ta). *Chemistry of Materials*, **2018**, 30, 392-402	9.6	7
89	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	3.8	9
88	Competition between Metal Dissolution and Gas Release in Li-Rich Li3RuyIr1−yO4 Model Compounds Showing Anionic Redox. *Chemistry of Materials*, **2018**, 30, 7682-7690	9.6	17
87	Reversible Sodium and Lithium Insertion in Iron Fluoride Perovskites. *Advanced Functional Materials* , **2018**, 28, 1802057	15.6	14
86	Chemical Activity of the Peroxide/Oxide Redox Couple: Case Study of BaRuO in Aqueous and Organic Solvents. *Chemistry of Materials*, **2018**, 30, 3882-3893	9.6	6
85	Evidence for anionic redox activity in a tridimensional-ordered Li-rich positive electrode Li2IrO. *Nature Materials*, **2017**, 16, 580-586	27	234
84	Requirements for reversible extra-capacity in Li-rich layered oxides for Li-ion batteries. *Energy and Environmental Science*, **2017**, 10, 266-274	35.4	192
83	Activation of surface oxygen sites on an iridium-based model catalyst for the oxygen evolution reaction. *Nature Energy*, **2017**, 2,	62.3	274
82	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	6.7	11
81	Approaching the limits of cationic and anionic electrochemical activity with the Li-rich layered rocksalt Li3IrO4. *Nature Energy*, **2017**, 2, 954-962	62.3	108
80	A2VO(SO4)2 (A = Li, Na) as Electrodes for Li-Ion and Na-Ion Batteries. *Chemistry of Materials*, **2016**, 28, 6637-6643	9.6	18
79	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	9.6	98
78	A Fully Ordered Triplite, LiCuSO4F. *Chemistry of Materials*, **2016**, 28, 1607-1610	9.6	5
77	The intriguing question of anionic redox in high-energy density cathodes for Li-ion batteries. *Energy and Environmental Science*, **2016**, 9, 984-991	35.4	346
76	Atomistic Modeling of Electrode Materials for Li-Ion Batteries: From Bulk to Interfaces. *Green Energy and Technology*, **2016**, 1-36	0.6	2

75	Origin of the Voltage Hysteresis of MgH2 Electrodes in Lithium Batteries. *Journal of Physical Chemistry C*, **2015**, 119, 17044-17052	3.8	35
74	Reversible Li-Intercalation through Oxygen Reactivity in Li-Rich Li-Fe-Te Oxide Materials. *Journal of the Electrochemical Society*, **2015**, 162, A1341-A1351	3.9	36
73	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	9.6	25
72	Origin of voltage decay in high-capacity layered oxide electrodes. *Nature Materials*, **2015**, 14, 230-8	27	612
71	Visualization of O-O peroxo-like dimers in high-capacity layered oxides for Li-ion batteries. *Science*, **2015**, 350, 1516-21	33.3	514
70	Influence of polymorphism on the electrochemical behavior of M Sb negative electrodes in Li/Na batteries. *Journal of Power Sources*, **2015**, 280, 695-702	8.9	17
69	New Insights on the Reversible Lithiation Mechanism of TiO2(B) by Operando X-ray Absorption Spectroscopy and X-ray Diffraction Assisted by First-Principles Calculations. *Journal of Physical Chemistry C*, **2014**, 118, 27210-27218	3.8	20
68	An oxysulfate Fe□(SO□)□ electrode for sustainable Li-based batteries. *Journal of the American Chemical Society*, **2014**, 136, 12658-66	16.4	14
67	Conceptual Surface Electrochemistry and New Redox Descriptors. *Journal of Physical Chemistry C*, **2014**, 118, 19023-19031	3.8	28
66	An intuitive and efficient method for cell voltage prediction of lithium and sodium-ion batteries. *Nature Communications*, **2014**, 5, 5559	17.4	33
65	Reversible anionic redox chemistry in high-capacity layered-oxide electrodes. *Nature Materials*, **2013**, 12, 827-35	27	969
64	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	5.3	52
63	High Performance Li2Ru1-yMnyO3 (0.2 ≤ y ≤ 0.8) Cathode Materials for Rechargeable Lithium-Ion Batteries: Their Understanding. *Chemistry of Materials*, **2013**, 25, 1121-1131	9.6	320
62	Palladium-silver mesowires for the extended detection of H2. *ACS Applied Materials & Interfaces*, **2013**, 5, 310-8	9.5	14
61	Origin of the Voltage Hysteresis in the CoP Conversion Material for Li-Ion Batteries. *Journal of Physical Chemistry C*, **2013**, 117, 837-849	3.8	76
60	Li(4)NiTeO(6) as a positive electrode for Li-ion batteries. *Chemical Communications*, **2013**, 49, 11376-8	5.8	71
59	Single-Step Synthesis of FeSO4F1-yOHy (0 ≤ y ≤ 1) Positive Electrodes for Li-Based Batteries. *Chemistry of Materials*, **2012**, 24, 1472-1485	9.6	31
58	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	35.4	54

57	Orbital Approach to the Electronic Structure of Solids **2012**,		19
56	A 3.90 V iron-based fluorosulphate material for lithium-ion batteries crystallizing in the triplite structure. *Nature Materials*, **2011**, 10, 772-9	27	279
55	Interface electrochemistry in conversion materials for Li-ion batteries. *Journal of Materials Chemistry*, **2011**, 21, 10134		61
54	FeII/FeIII 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	8.9	46
53	Crystal structure, band structure and electrical properties of □(BEDT-TTF)2SbF6 grown on a Si(0 0 1) electrode. *Synthetic Metals*, **2010**, 160, 556-560	3.6	3
52	Design of Electrode Materials for Lithium-Ion Batteries: The Example of Metal□Organic Frameworks. *Journal of Physical Chemistry C*, **2010**, 114, 9518-9527	3.8	75
51	Interplay between Magnetic and Orbital Ordering in the Strongly Correlated Cobalt Oxide: A DFT + U Study. *Journal of Physical Chemistry C*, **2010**, 114, 21750-21756	3.8	28
50	P-Redox Mechanism at the Origin of the High Lithium Storage in NiP2-Based Batteries. *Chemistry of Materials*, **2009**, 21, 298-308	9.6	66
49	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	3.9	94
48	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	3.8	35
47	Direct Correlation between the 31P MAS NMR Response and the Electronic Structure of Some Transition Metal Phosphides. *Journal of Physical Chemistry C*, **2008**, 112, 20481-20490	3.8	44
46	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	2.7	31
45	Redox mechanism in the NiP2 electrode for Li-ion batteries: A DFT study coupled with local chemical bond analyses. *Ionics*, **2008**, 14, 197-202	2.7	6
44	Determination of Lithium Insertion Sites in LixTiP4(x= 2□1) by Electron Energy-Loss Spectroscopy. *Journal of Physical Chemistry C*, **2007**, 111, 3996-4002	3.8	19
43	Electrical conductivity and spin crossover: a new achievement with a metal bis dithiolene complex. *Inorganic Chemistry*, **2007**, 46, 8548-59	5.1	96
42	Mixed-valence li/fe-based metal-organic frameworks with both reversible redox and sorption properties. *Angewandte Chemie - International Edition*, **2007**, 46, 3259-63	16.4	518
41	(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	1.3	1
40	FeP: Another Attractive Anode for the Li-Ion Battery Enlisting a Reversible Two-Step Insertion/Conversion Process. *Chemistry of Materials*, **2006**, 18, 3531-3538	9.6	165

39	Redox mechanism in the binary transition metal phosphide Cu3P. *Journal of Physics and Chemistry of Solids*, **2006**, 67, 1252-1257	3.9	43
38	(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	1.3	
37	On the Reactivity of Li8-yMnyP4 toward Lithium. *Chemistry of Materials*, **2005**, 17, 3627-3635	9.6	31
36	Electrochemical Reactivity and Design of NiP2 Negative Electrodes for Secondary Li-Ion Batteries. *Chemistry of Materials*, **2005**, 17, 6327-6337	9.6	209
35	Electrochemical Behaviors of Binary and Ternary Manganese Phosphides. *Chemistry of Materials*, **2005**, 17, 5817-5823	9.6	54
34	Progress in the lithium insertion mechanism in Cu3P. *Ionics*, **2005**, 11, 36-45	2.7	18
33	Leading interactions in the SrV6O15 compound. *Physical Review B*, **2005**, 71,	3.3	33
32	The LixMPn4 phases (M/Pn = Ti/P, V/As): new negative electrode materials for lithium ion rechargeable batteries. *Electrochimica Acta*, **2004**, 49, 2325-2332	6.7	49
31	Redox-Induced Structural Change in Anode Materials Based on Tetrahedral (MPn4)x- Transition Metal Pnictides. *Chemistry of Materials*, **2004**, 16, 1002-1013	9.6	57
30	Lithium insertion/deinsertion mechanisms in the transition metal pnictides LixMPn4. *Ionics*, **2003**, 9, 56-63	2.7	9
29	New salts derived from organic donor molecules with long-living excited states counter-ions. *Synthetic Metals*, **2003**, 133-134, 377-380	3.6	1
28	Similarities between the t-J and Hubbard models in weakly correlated regimes. *European Physical Journal B*, **2002**, 28, 49-54	1.2	1
27	The LixVPn4 Ternary Phases (Pn = P, As): Rigid Networks for Lithium Intercalation/Deintercalation. *Chemistry of Materials*, **2002**, 14, 4126-4133	9.6	56
26	Structure and properties of BETS salts: (BETS)8(Cu2Cl6)(CuCl4), (BETS)2(CuCl2) and (BETS)2(CuCl4). *Comptes Rendus De L'Academie Des Sciences - Series IIc: Chemistry*, **2001**, 4, 149-160		0
25	Anion Conformation and Physical Properties in BETS Salts with the Nitroprusside Anion and its Related Ruthenium Halide (X = Cl, Br) Mononitrosyl Complexes: (BETS)4[Fe(CN)5NO], (BETS)2[RuBr5NO], and (BETS)2[RuCl5NO]. *European Journal of Inorganic Chemistry*, **2001**, 2001, 2797	2.3	23
24	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		8
23	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	3.9	22
22	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 model. *Journal of Chemical Physics*, **1999**, 110, 1767-1773	3.9	6

21	Why has 1T-TaTe2 not yet been synthetized? A DFT contribution.. *Synthetic Metals*, **1999**, 103, 2679-2682	3.6	2
20	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	3.6	
19	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	3.9	10
18	Metallic conductivity in a disordered charge-transfer salt derived from cis-BET-TTF. *Synthetic Metals* , **1997**, 86, 2145-2146	3.6	12
17	Electronic Structure of the $mathsf{alpha}$-(BEDT-TTF)$mathsf{_2}$MHg(XCN)$mathsf{_4}$ (M = Tl, K, NH$mathsf{_4}$; X = S, Se) and Related Phases. Synthesis and Crystal Structure of the New Stable Organic Metal $alpha$-(BEDT-TTF)$mathsf{_2}$TlHg(Se$mathsf{_{rm 1-x}}$S$mathsf{_{rm x}}$CN)$mathsf{_4}$ (x = 0.125). *Journal De Physique, I*, **1996**, 6, 1527-1553		29
16	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	2.8	2
15	H2O photodissociation dynamics based on potential energy surfaces from density functional calculations. *Journal of Chemical Physics*, **1995**, 103, 2538-2547	3.9	12
14	Structural and electronic properties of the molecular conductors (EDTTTF)x[Pd(dmit)2]y(x:y=2:3 and 2:2). *Journal of Physics Condensed Matter*, **1995**, 7, 4673-4695	1.8	11
13	A New Family of Molecular Metals Based on Bis(ethylenethio)tetrathiafulvalene (BET-TTF) and Octahedral Counterions. *Chemistry of Materials*, **1995**, 7, 1558-1567	9.6	23
12	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	3.6	4
11	Magnetoresistance in pulsed fields, band structure calculations and charge-density wave instability in (TSeT)2Cl. *Synthetic Metals*, **1995**, 70, 1279-1280	3.6	4
10	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	3.6	3
9	Concerning the first-order transition in the ?-phase (BEDT-TTF)4PtCl6 . C6H5CN. *Journal De Physique, I*, **1994**, 4, 1479-1490		20
8	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		8
7	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	16.4	14
6	The Mechanism of Acetylene Cyclotrimerization Catalyzed by the fac-IrP3+ Fragment: The Relationship between Fluxionality and Catalysis. *Organometallics*, **1994**, 13, 2010-2023	3.8	50
5	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	5.1	38
4	Inhibited superconductivity induced by localization effects in (EDT-TTF)2[Pd(dmit)2]2. *Synthetic Metals*, **1993**, 56, 2833-2838	3.6	5

3	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	1.6	22
2	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		4
1	The IrOOOOIr transition state and the mechanism of the oxygen evolution reaction on IrO2(110). *Energy and Environmental Science*,	35.4	7