Manuel Smeu

List of Publications by Year
in descending order

46 papers	1,249 citations	361413 20 h-index	377865 34 g-index
47 all docs	47 docs citations	47 times ranked	1845 citing authors

#	Article	IF	Citations
1	2D Ni0.25Mn0.75O2: A high-performance cathode for multivalent ion batteries. Computational Materials Science, 2022, 202, 110948.	3.0	4
2	Beyond Simple Structureâ€“Function Relationships: The Interplay of Geometry, Electronic Structure, and Molecule/Electrode Coupling in Single-Molecule Junctions. Journal of Physical Chemistry C, 2022, 126, 6653-6661.	3.1	3
3	Electron leakage through heterogeneous LiF on lithiumâ€“metal battery anodes. Physical Chemistry Chemical Physics, 2021, 23, 3214-3218.	2.8	22
4	Correlated Energy-Level Alignment Effects Determine Substituent-Tuned Single-Molecule Conductance. ACS Applied Materials & Interfaces, 2021, 13, 4267-4277.	8.0	11
5	Ab Initio Investigation of the Elastic Properties of CaxSn1â^’x Alloys for Use As Battery Anodes. Journal of Electrochemical Energy Conversion and Storage, 2021, 18, .	2.1	5
6	Preventing Electrolyte Decomposition on a Ca Metal Electrode Interface Using an Artificial Solidâ€Electrolyte Interphase. Advanced Theory and Simulations, 2021, 4, 2100018.	2.8	7
7	Phenalenyls as tunable excellent molecular conductors and switchable spin filters. Physical Chemistry Chemical Physics, 2021, 23, 24106-24110.	2.8	10
8	A Computational Comparison of Ether and Ester Electrolyte Stability on a Ca Metal Anode. Energy Material Advances, 2021, 2021, .	11.0	11
9	First principles investigation into the interwoven nature of voltage and mechanical properties of the Li<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e95" altimg="si118.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>NMC-811 cathode. Journal of Power Sources, 2021, 516, 230620.	7.8	10
10	Ab initio investigation of Î±- and Î¶-V2O5 for beyond lithium ion battery cathodes. Journal of Power Sources, 2020, 472, 228096.	7.8	17
11	Reassessing destructive quantum interference in azulene-based devices. Physical Chemistry Chemical Physics, 2020, 22, 3653-3660.	2.8	5
12	Combined Impact of Denticity and Orientation on Molecular-Scale Charge Transport. Journal of Physical Chemistry C, 2020, 124, 9460-9469.	3.1	4
13	Ab initio investigation of the temperature-dependent elastic properties of Bi, Te and Cu. Journal of Physics Condensed Matter, 2020, 32, 485902.	1.8	5
14	TiSe2 cathode for beyond Li-ion batteries. Journal of Power Sources, 2019, 436, 226813.	7.8	36
15	Ab initio investigation of the elastic properties of bismuth-based alloys. Physical Review B, 2019, 100, .	3.2	15
16	First principles study of graphene on metals with the SCAN and SCAN+rVV10 functionals. Journal of Chemical Physics, 2019, 150, 154702.	3.0	17
17	Atomistic simulation of the structural and conductance evolution of Au break junctions. Computational Materials Science, 2019, 164, 147-152.	3.0	1
18	Comparative Study of Ethylene Carbonate-Based Electrolyte Decomposition at Li, Ca, and Al Anode Interfaces. ACS Applied Energy Materials, 2019, 2, 1676-1684.	5.1	36

#	Article	IF	Citations
19	Ab initio investigation into the physisorption of noble gases on graphene. Surface Science, 2019, 682, 38-42.	1.9	12
20	Ba₄B₈TeO₁₉: A UV Nonlinear Optical Material. Inorganic Chemistry, 2018, 57, 4771-4776.	4.0	31
21	Density Functional Theory Modeling of MnO₂ Polymorphs as Cathodes for Multivalent Ion Batteries. Journal of Physical Chemistry C, 2018, 122, 8788-8795.	3.1	70
22	Ab initio study of structural and electronic properties of copper and nickel tungstate. Computational Materials Science, 2018, 143, 301-307.	3.0	9
23	Ethylene Carbonate-Based Electrolyte Decomposition and Solidâ€“Electrolyte Interphase Formation on Ca Metal Anodes. Journal of Physical Chemistry Letters, 2018, 9, 3295-3300.	4.6	29
24	Spin-Negative Differential Resistance in Zigzag Graphene Nanoribbons with Side-Attached Porphine Molecule. Journal of Physical Chemistry C, 2018, 122, 15911-15921.	3.1	14
25	Tuning the electronic and quantum transport properties of nitrogenated holey graphene nanoribbons. Journal of Materials Chemistry C, 2017, 5, 11856-11866.	5.5	13
26	Hybrid density functional theory modeling of Ca, Zn, and Al ion batteries using the Chevrel phase Mo₆S₈ cathode. Physical Chemistry Chemical Physics, 2017, 19, 20684-20690.	2.8	41
27	Two-Dimensional Î³-Graphyne Suspended on Si(111): A Hybrid Device. Journal of Physical Chemistry C, 2016, 120, 4605-4611.	3.1	16
28	Theoretical investigation of Chevrel phase materials for cathodes accommodating Ca2+ ions. Journal of Power Sources, 2016, 306, 431-436.	7.8	58
29	Towards graphyne molecular electronics. Nature Communications, 2015, 6, 6321.	12.8	135
30	Singleâ€Molecule Sensing of Environmental pHâ€”an STM Break Junction and NEGFâ€DFT Approach. Angewandte Chemie - International Edition, 2014, 53, 1098-1102.	13.8	82
31	Modeling ion sensing in molecular electronics. Journal of Chemical Physics, 2014, 140, 054709.	3.0	11
32	Hapticity-Dependent Charge Transport through Carbodithioate-Terminated [5,15-Bis(phenylethynyl)porphinato]zinc(II) Complexes in Metalâ€“Moleculeâ€“Metal Junctions. Nano Letters, 2014, 14, 5493-5499.	9.1	29
33	Molecular Junctions: Can Pulling Influence Optical Controllability?. Nano Letters, 2014, 14, 4587-4591.	9.1	22
34	Molecular Spintronics: Destructive Quantum Interference Controlled by a Gate. Journal of the American Chemical Society, 2014, 136, 15065-15071.	13.7	65
35	Conductivity of Si(111)-(<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq1 1 0.784314 rgBT /Overlock 10 T The Role of a Single Atomic Step. Physical Review Letters, 2014, 112, 246802.	7.8	30
36	Effect of Anchoring Groups on Single Molecule Charge Transport through Porphyrins. Journal of Physical Chemistry C, 2013, 117, 14890-14898.	3.1	88

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37	Spin Transport of Polyacetylene Chains Bridging Zigzag Graphene Nanoribbon Electrodes: A Nonequilibrium Treatment of Structural Control and Spin Filtering. Journal of Physical Chemistry C, 2013, 117, 21178-21185.	3.1	16
38	Electronic properties of Si(111)-7Ã—7and related reconstructions: Density functional theory calculations. Physical Review B, 2012, 85, .	3.2	28
39	Conduction modulation of Ï€-stacked ethylbenzene wires on Si(100) with substituent groups. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	9
40	Conduction modulation of Ï€-stacked ethylbenzene wires on Si(100) with substituent groups. , 2012, , 37-44.		0
41	Energetic Molecules Encapsulated Inside Carbon Nanotubes and between Graphene Layers: DFT Calculations. Journal of Physical Chemistry C, 2011, 115, 10985-10989.	3.1	60
42	Calculations of Electron Transport through Simple Ï€- and Ï*f*-Type Radicals. Journal of Physical Chemistry C, 2010, 114, 17874-17879.	3.1	36
43	Conduction Pathway of Ï€-Stacked Ethylbenzene Molecular Wires on Si(100). Journal of the American Chemical Society, 2009, 131, 11019-11026.	13.7	34
44	Theoretical investigation of electron transport modulation through benzenedithiol by substituent groups. Journal of Chemical Physics, 2008, 129, 034707.	3.0	20
45	Rearrangement of the 1,1-Diphenylethoxyl Radical Is Not Concerted but Occurs through a Bridged Intermediate. Journal of Organic Chemistry, 2007, 72, 4520-4523.	3.2	18
46	Isomerization of Triphenylmethoxyl and 1,1-Diphenylethoxyl Radicals. Revised Assignment of the Electron-Spin Resonance Spectra of Purported Intermediates Formed during the Ceric Ammonium Nitrate Mediated Photooxidation of Aryl Carbinols. Journal of Organic Chemistry, 2006, 71, 9906-9908.	3.2	23