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	Towards graphyne molecular electronics. Nature Communications, 2015, 6, 6321.	12.8	135
2	Effect of Anchoring Groups on Single Molecule Charge Transport through Porphyrins. Journal of Physical Chemistry C, 2013, 117, 14890-14898.	3.1	88
3	Singleâ€Molecule Sensing of Environmental pHâ€”an STM Break Junction and NEGFâ€ĐFT Approach. Angewandte Chemie - International Edition, 2014, 53, 1098-1102.	13.8	82
4	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
5	Molecular Spintronics: Destructive Quantum Interference Controlled by a Gate. Journal of the American Chemical Society, 2014, 136, 15065-15071.	13.7	65
6	Energetic Molecules Encapsulated Inside Carbon Nanotubes and between Graphene Layers: DFT Calculations. Journal of Physical Chemistry C, 2011, 115, 10985-10989.	3.1	60
7	Theoretical investigation of Chevrel phase materials for cathodes accommodating Ca2+ ions. Journal of Power Sources, 2016, 306, 431-436.	7.8	58
8	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
9	Calculations of Electron Transport through Simple Ï€- and Ïƒ-Type Radicals. Journal of Physical Chemistry C, 2010, 114, 17874-17879.	3.1	36
10	TiSe2 cathode for beyond Li-ion batteries. Journal of Power Sources, 2019, 436, 226813.	7.8	36
11	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
12	Conduction Pathway of Ï€-Stacked Ethylbenzene Molecular Wires on Si(100). Journal of the American Chemical Society, 2009, 131, 11019-11026.	13.7	34
13	Ba₄B₈TeO₁₉: A UV Nonlinear Optical Material. Inorganic Chemistry, 2018, 57, 4771-4776.	4.0	31
14	Conductivity of Si(111)-(<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 227 T The Role of a Single Atomic Step. Physical Review Letters, 2014, 112, 246802.	7.8	30
15	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
16	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
17	Electronic properties of Si(111)-7Ã—7and related reconstructions: Density functional theory calculations. Physical Review B, 2012, 85, .	3.2	28
18	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

#	Article	IF	Citations
19	Molecular Junctions: Can Pulling Influence Optical Controllability?. Nano Letters, 2014, 14, 4587-4591.	9.1	22
20	Electron leakage through heterogeneous LiF on lithiumâ€“metal battery anodes. Physical Chemistry Chemical Physics, 2021, 23, 3214-3218.	2.8	22
21	Theoretical investigation of electron transport modulation through benzenedithiol by substituent groups. Journal of Chemical Physics, 2008, 129, 034707.	3.0	20
22	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
23	First principles study of graphene on metals with the SCAN and SCAN+rVV10 functionals. Journal of Chemical Physics, 2019, 150, 154702.	3.0	17
24	Ab initio investigation of Î±- and Î¶-V2O5 for beyond lithium ion battery cathodes. Journal of Power Sources, 2020, 472, 228096.	7.8	17
25	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
26	Two-Dimensional Î³-Graphyne Suspended on Si(111): A Hybrid Device. Journal of Physical Chemistry C, 2016, 120, 4605-4611.	3.1	16
27	Ab initio investigation of the elastic properties of bismuth-based alloys. Physical Review B, 2019, 100, .	3.2	15
28	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
29	Tuning the electronic and quantum transport properties of nitrogenated holey graphene nanoribbons. Journal of Materials Chemistry C, 2017, 5, 11856-11866.	5.5	13
30	Ab initio investigation into the physisorption of noble gases on graphene. Surface Science, 2019, 682, 38-42.	1.9	12
31	Modeling ion sensing in molecular electronics. Journal of Chemical Physics, 2014, 140, 054709.	3.0	11
32	Correlated Energy-Level Alignment Effects Determine Substituent-Tuned Single-Molecule Conductance. ACS Applied Materials & Interfaces, 2021, 13, 4267-4277.	8.0	11
33	A Computational Comparison of Ether and Ester Electrolyte Stability on a Ca Metal Anode. Energy Material Advances, 2021, 2021, .	11.0	11
34	Phenalenyls as tunable excellent molecular conductors and switchable spin filters. Physical Chemistry Chemical Physics, 2021, 23, 24106-24110.	2.8	10
35	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
36	Conduction modulation of Ï€-stacked ethylbenzene wires on Si(100) with substituent groups. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	9

#	Article	IF	Citations
37	Ab initio study of structural and electronic properties of copper and nickel tungstate. Computational Materials Science, 2018, 143, 301-307.	3.0	9
38	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
39	Reassessing destructive quantum interference in azulene-based devices. Physical Chemistry Chemical Physics, 2020, 22, 3653-3660.	2.8	5
40	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
41	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
42	Combined Impact of Denticity and Orientation on Molecular-Scale Charge Transport. Journal of Physical Chemistry C, 2020, 124, 9460-9469.	3.1	4
43	2D Ni0.25Mn0.75O2: A high-performance cathode for multivalent ion batteries. Computational Materials Science, 2022, 202, 110948.	3.0	4
44	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
45	Atomistic simulation of the structural and conductance evolution of Au break junctions. Computational Materials Science, 2019, 164, 147-152.	3.0	1
46	Conduction modulation of Ï€-stacked ethylbenzene wires on Si(100) with substituent groups. , 2012, , 37-44.		0