Roel S Sanchez-Carrera

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/10763929/publications.pdf

Version: 2024-02-01

23 papers	3,074 citations	430843 18 h-index	677123 22 g-index
23 all docs	23 docs citations	23 times ranked	4645 citing authors

#	Article	IF	Citations
1	Microkinetic Modeling of Propene Combustion on a Stepped, Metallic Palladium Surface and the Importance of Oxygen Coverage. ACS Catalysis, 2022, 12, 1742-1757.	11.2	13
2	Insights and comparison of structureâ€“property relationships in propane and propene catalytic combustion on Pd- and Pt-based catalysts. Journal of Catalysis, 2021, 401, 89-101.	6.2	24
3	Revealing the structure of a catalytic combustion active-site ensemble combining uniform nanocrystal catalysts and theory insights. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 14721-14729.	7.1	16
4	Modeling the Migration of Platinum Nanoparticles on Surfaces Using a Kinetic Monte Carlo Approach. Journal of Physical Chemistry C, 2017, 121, 4261-4269.	3.1	29
5	Modeling the Interface of Platinum and Î±-Quartz(001): Implications for Sintering. Journal of Physical Chemistry C, 2016, 120, 10340-10350.	3.1	18
6	Computational Raman spectroscopy of organometallic reaction products in lithium and sodium-based battery systems. Physical Chemistry Chemical Physics, 2014, 16, 24549-24558.	2.8	13
7	Accelerated computational discovery of high-performance materials for organic photovoltaics by means of cheminformatics. Energy and Environmental Science, 2011, 4, 4849.	30.8	169
8	From computational discovery to experimental characterization of a high hole mobility organic crystal. Nature Communications, 2011, 2, 437.	12.8	321
9	The Harvard Clean Energy Project: Large-Scale Computational Screening and Design of Organic Photovoltaics on the World Community Grid. Journal of Physical Chemistry Letters, 2011, 2, 2241-2251.	4.6	470
10	A Critical Review of Li/Air Batteries. Journal of the Electrochemical Society, 2011, 159, R1-R30.	2.9	950
11	Optical absorption and emission properties of end-capped oligothienoacenes: A joint theoretical and experimental study. Organic Electronics, 2010, 11, 1701-1712.	2.6	19
12	Failure of Conventional Density Functionals for the Prediction of Molecular Crystal Polymorphism: A Quantum Monte Carlo Study. Journal of Physical Chemistry Letters, 2010, 1, 1789-1794.	4.6	61
13	Electronic Properties of the 2,6-Diiododithieno[3,2-b:2â€²,3â€²-d]thiophene Molecule and Crystal: A Joint Experimental and Theoretical Study. Journal of Physical Chemistry B, 2010, 114, 749-755.	2.6	21
14	Influence of Structural Dynamics on Polarization Energies in Anthracene Single Crystals. Journal of Physical Chemistry C, 2010, 114, 20678-20685.	3.1	86
15	Theoretical Characterization of the Air-Stable, High-Mobility Dinaphtho[2,3-b:2â€²3â€²-f]thieno[3,2-b]-thiophene Organic Semiconductor. Journal of Physical Chemistry C, 2010, 114, 2334-2340.	3.1	73
16	Interaction of Charge Carriers with Lattice Vibrations in Oligoacene Crystals from Naphthalene to Pentacene. Journal of the American Chemical Society, 2010, 132, 14437-14446.	13.7	128
17	Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene. ChemPhysChem, 2009, 10, 2265-2273.	2.1	77
18	Inside Cover: Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene (ChemPhysChem 13/2009). ChemPhysChem, 2009, 10, 2158-2158.	2.1	0

#	Article	IF	Citations
19	Impact of Perfluorination on the Charge-Transport Parameters of Oligoacene Crystals. Journal of the American Chemical Society, 2009, 131, 1502-1512.	13.7	174
20	Interaction of Charge Carriers with Lattice Vibrations in Organic Molecular Semiconductors: Naphthalene as a Case Study. Journal of Physical Chemistry C, 2009, 113, 4679-4686.	3.1	102
21	Charge-Transport Properties of the 1,4-Diiodobenzene Crystal: A Quantum-Mechanical Study. Chemistry of Materials, 2008, 20, 5832-5838.	6.7	17
22	Charge Transport Parameters of the Pentathienoacene Crystal. Journal of the American Chemical Society, 2007, 129, 13072-13081.	13.7	153
23	Vibronic Coupling in the Ground and Excited States of Oligoacene Cationsâ€. Journal of Physical Chemistry B, 2006, 110, 18904-18911.	2.6	140