Ask Hjorth Larsen

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Real-time time-dependent density functional theory implementation of electronic circular dichroism applied to nanoscale metal–organic clusters. Journal of Chemical Physics, 2021, 154, 114102.	3.0	16
2	Recent progress of the Computational 2D Materials Database (C2DB). 2D Materials, 2021, 8, 044002.	4.4	218
3	Spread-balanced Wannier functions: Robust and automatable orbital localization. Physical Review B, 2021, 104, .	3.2	3
4	Atomic Simulation Recipes: A Python framework and library for automated workflows. Computational Materials Science, 2021, 199, 110731.	3.0	35
5	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
6	Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems. Journal of Chemical Physics, 2020, 152, 124119.	3.0	210
7	Optical excitations of chlorophyll <i>a</i> and <i>b</i> monomers and dimers. Journal of Chemical Physics, 2019, 151, 174102.	3.0	9
8	Intrinsic core level photoemission of suspended monolayer graphene. Physical Review Materials, 2018, 2, .	2.4	15
9	libvdwxc: a library for exchange–correlation functionals in the vdW-DF family. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 065004.	2.0	28
10	The atomic simulation environment—a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	1.8	1,933
11	Dynamical Processes in Open Quantum Systems from a TDDFT Perspective: Resonances and Electron Photoemission. Topics in Current Chemistry, 2015, 368, 219-271.	4.0	3
12	Modeling electron dynamics coupled to continuum states in finite volumes with absorbing boundaries. European Physical Journal B, 2015, 88, 1.	1.5	64
13	Real-space grids and the Octopus code as tools for the development of new simulation approaches for electronic systems. Physical Chemistry Chemical Physics, 2015, 17, 31371-31396.	2.8	376
14	Climbing the Activity Volcano: Core–Shell Ru@Pt Electrocatalysts for Oxygen Reduction. ChemElectroChem, 2014, 1, 67-71.	3.4	49
15	Investigation of Catalytic Finite-Size-Effects of Platinum Metal Clusters. Journal of Physical Chemistry Letters, 2013, 4, 222-226.	4.6	249
16	Stark Ionization of Atoms and Molecules within Density Functional Resonance Theory. Journal of Physical Chemistry Letters, 2013, 4, 2734-2738.	4.6	18
17	Balance of Nanostructure and Bimetallic Interactions in Pt Model Fuel Cell Catalysts: In Situ XAS and DFT Study. Journal of the American Chemical Society, 2012, 134, 9664-9671.	13.7	117
18	Finite Size Effects in Chemical Bonding: From Small Clusters to Solids. Catalysis Letters, 2011, 141, 1067-1071.	2.6	234

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#	Article	IF	CITATIONS
19	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. Journal of Physics Condensed Matter, 2010, 22, 253202.	1.8	1,451