Ask Hjorth Larsen

List of Publications by Year
in descending order

19	5,047	567281 15	794594 19
papers	citations	h-index	g-index

19	19	19	6718
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The atomic simulation environmentâ€”a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	1.8	1,933
2	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
3	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
4	Investigation of Catalytic Finite-Size-Effects of Platinum Metal Clusters. Journal of Physical Chemistry Letters, 2013, 4, 222-226.	4.6	249
5	Finite Size Effects in Chemical Bonding: From Small Clusters to Solids. Catalysis Letters, 2011, 141, 1067-1071.	2.6	234
6	Recent progress of the Computational 2D Materials Database (C2DB). 2D Materials, 2021, 8, 044002.	4.4	218
7	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
8	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
9	Modeling electron dynamics coupled to continuum states in finite volumes with absorbing boundaries. European Physical Journal B, 2015, 88, 1.	1.5	64
10	Climbing the Activity Volcano: Coreâ€“Shell Ru@Pt Electrocatalysts for Oxygen Reduction. ChemElectroChem, 2014, 1, 67-71.	3.4	49
11	Atomic Simulation Recipes: A Python framework and library for automated workflows. Computational Materials Science, 2021, 199, 110731.	3.0	35
12	libvdwxc: a library for exchangeâ€“correlation functionals in the vdW-DF family. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 065004.	2.0	28
13	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
14	Stark Ionization of Atoms and Molecules within Density Functional Resonance Theory. Journal of Physical Chemistry Letters, 2013, 4, 2734-2738.	4.6	18
15	Real-time time-dependent density functional theory implementation of electronic circular dichroism applied to nanoscale metalâ€“organic clusters. Journal of Chemical Physics, 2021, 154, 114102.	3.0	16
16	Intrinsic core level photoemission of suspended monolayer graphene. Physical Review Materials, 2018, 2, .	2.4	15
17	Optical excitations of chlorophyll a and b monomers and dimers. Journal of Chemical Physics, 2019, 151, 174102.	3.0	9
18	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

#	Article	IF	Citations
19	Spread-balanced Wannier functions: Robust and automatable orbital localization. Physical Review B, 2021, 104, .	3.2	3