Mathias Ljungberg

List of Publications by Year
in descending order

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28	2,996	430874 18	501196 28
papers	citations	h-index	g-index

29	29	29	4083
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	The inhomogeneous structure of water at ambient conditions. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15214-15218.	7.1	526
3	Theoretical approximations to X-ray absorption spectroscopy of liquid water and ice. Journal of Electron Spectroscopy and Related Phenomena, 2010, 177, 135-157.	1.7	132
4	Diffraction and IR/Raman data do not prove tetrahedral water. Journal of Chemical Physics, 2008, 129, 084502.	3.0	94
5	First-principles model potentials for lattice-dynamical studies: general methodology and example of application to ferroic perovskite oxides. Journal of Physics Condensed Matter, 2013, 25, 305401.	1.8	90
6	On the Range of Water Structure Models Compatible with X-ray and Neutron Diffraction Data. Journal of Physical Chemistry B, 2009, 113, 6246-6255.	2.6	81
7	Core level binding energies of functionalized and defective graphene. Beilstein Journal of Nanotechnology, 2014, 5, 121-132.	2.8	70
8	An implementation of core level spectroscopies in a real space Projector Augmented Wave density functional theory code. Journal of Electron Spectroscopy and Related Phenomena, 2011, 184, 427-439.	1.7	61
9	Are recent water models obtained by fitting diffraction data consistent with infrared/Raman and x-ray absorption spectra?. Journal of Chemical Physics, 2006, 125, 244510.	3.0	60
10	Vibrational interference effects in x-ray emission of a model water dimer: Implications for the interpretation of the liquid spectrum. Journal of Chemical Physics, 2011, 134, 044513.	3.0	46
11	Resonant inelastic X-ray scattering of liquid water. Journal of Electron Spectroscopy and Related Phenomena, 2013, 188, 84-100.	1.7	45
12	Reply to Soper et al.: Fluctuations in water around a bimodal distribution of local hydrogen-bonded structural motifs. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, .	7.1	44
13	A phononic switch based on ferroelectric domain walls. Physical Review B, 2017, 96, .	3.2	39
14	Cubic-scaling iterative solution of the Bethe-Salpeter equation for finite systems. Physical Review B, 2015, 92, .	3.2	37
15	Calculation of the graphene C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>s</mml:mi></mml:mrow></mml:math> core level binding energy. Physical Review B, 2015, 91, .	3.2	36
16	Semiclassical description of nuclear dynamics in x-ray emission of water. Physical Review B, 2010, 82, .	3.2	34
17	Complementarity between high-energy photoelectron and L-edge spectroscopy for probing the electronic structure of 5d transition metal catalysts. Physical Chemistry Chemical Physics, 2010, 12, 5694.	2.8	23
18	X-ray emission spectroscopy and density functional study of CO/Fe(100). Journal of Chemical Physics, 2012, 136, 034702.	3.0	21

#	Article	IF	Citations
19	Assessment of Density-Functional Tight-Binding Ionization Potentials and Electron Affinities of Molecules of Interest for Organic Solar Cells Against First-Principles GW Calculations. Computation, 2015, 3, 616-656.	2.0	19
20	Core-hole-induced dynamical effects in the x-ray emission spectrum of liquid methanol. Journal of Chemical Physics, 2017, 146, 134506.	3.0	18
21	X-ray Emission Spectrum of Liquid Ethanol: Origin of Split Peaks. Journal of Physical Chemistry B, 2017, 121, 11163-11168.	2.6	15
22	Charge-transfer states and optical transitions at the pentacene-TiO₂interface. New Journal of Physics, 2017, 19, 033019.	2.9	13
23	Assessing the electric-field approximation to IR and Raman spectra of dilute HOD in D2O. Journal of Chemical Physics, 2009, 131, 034501.	3.0	11
24	Vibrational effects in x-ray absorption and resonant inelastic x-ray scattering using a semiclassical scheme. Physical Review B, 2017, 96, .	3.2	8
25	Temperature-Dependent Classical Phonons from Efficient Nondynamical Simulations. Physical Review Letters, 2013, 110, 105503.	7.8	6
26	Stability of Pt-Modified Cu(111) in the Presence of Oxygen and Its Implication on the Overall Electronic Structure. Journal of Physical Chemistry C, 2013, 117, 16371-16380.	3.1	5
27	Computation of electron energy loss spectra by an iterative method. Nuclear Instruments & Methods in Physics Research B, 2015, 354, 216-219.	1.4	5
28	Hybrid cluster-expansion and density-functional-theory approach for optical absorption in TiO_2. Journal of the Optical Society of America B: Optical Physics, 2016, 33, C123.	2.1	4