Mathias Ljungberg

List of Publications by Year
in descending order

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	Core-hole-induced dynamical effects in the x-ray emission spectrum of liquid methanol. Journal of Chemical Physics, 2017, 146, 134506.	3.0	18
2	Charge-transfer states and optical transitions at the pentacene-TiO₂interface. New Journal of Physics, 2017, 19, 033019.	2.9	13
3	A phononic switch based on ferroelectric domain walls. Physical Review B, 2017, 96, .	3.2	39
4	Vibrational effects in x-ray absorption and resonant inelastic x-ray scattering using a semiclassical scheme. Physical Review B, 2017, 96, .	3.2	8
5	X-ray Emission Spectrum of Liquid Ethanol: Origin of Split Peaks. Journal of Physical Chemistry B, 2017, 121, 11163-11168.	2.6	15
6	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
7	Cubic-scaling iterative solution of the Bethe-Salpeter equation for finite systems. Physical Review B, 2015, 92, .	3.2	37
8	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
9	Computation of electron energy loss spectra by an iterative method. Nuclear Instruments & Methods in Physics Research B, 2015, 354, 216-219.	1.4	5
10	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:m level binding energy. Physical Review B, 2015, 91, .	3.2	36
11	Core level binding energies of functionalized and defective graphene. Beilstein Journal of Nanotechnology, 2014, 5, 121-132.	2.8	70
12	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
13	Resonant inelastic X-ray scattering of liquid water. Journal of Electron Spectroscopy and Related Phenomena, 2013, 188, 84-100.	1.7	45
14	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
15	Temperature-Dependent Classical Phonons from Efficient Nondynamical Simulations. Physical Review Letters, 2013, 110, 105503.	7.8	6
16	X-ray emission spectroscopy and density functional study of CO/Fe(100). Journal of Chemical Physics, 2012, 136, 034702.	3.0	21
17	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
18	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

#	Article	IF	Citations
19	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
20	Semiclassical description of nuclear dynamics in x-ray emission of water. Physical Review B, 2010, 82, .	3.2	34
21	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
22	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
23	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
24	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
25	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
26	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
27	Diffraction and IR/Raman data do not prove tetrahedral water. Journal of Chemical Physics, 2008, 129, 084502.	3.0	94
28	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