Andreas Pedersen

List of Publications by Year
in descending order

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34 papers	1,059 citations	516561 16 h-index	477173 29 g-index
34 all docs	34 docs citations	34 times ranked	1631 citing authors

#	Article	IF	Citations
1	Reassignment of magic numbers for icosahedral Au clusters: 310, 564, 928 and 1426. Nanoscale, 2022, 14, 9053-9060.	2.8	3
2	Atomic and electronic structures of a vacancy in amorphous silicon. Physical Review B, 2020, 101, .	1.1	6
3	Reassignment of â€˜magic numbersâ€™ for Au clusters of decahedral and FCC structural motifs. Nanoscale, 2018, 10, 5124-5132.	2.8	23
4	Optimal atomic structure of amorphous silicon obtained from density functional theory calculations. New Journal of Physics, 2017, 19, 063018.	1.2	32
5	Electronic properties of lithiated SnO-based anode materials. Journal of Applied Physics, 2017, 122, 055105.	1.1	2
6	Lithiation of Silicon Nanoclusters. Physical Review Applied, 2017, 7, .	1.5	9
7	Diffusion mechanisms in Li0.5CoO2â€”A computational study. Applied Physics Letters, 2016, 108, 153902.	1.5	3
8	Atomistic simulation of nanodevices. , 2016, , .		5
9	Atomic scale plasmonic devices. , 2016, , .		0
10	Atomic Scale Plasmonic Switch. Nano Letters, 2016, 16, 709-714.	4.5	118
11	Three-Phase Model for the Reversible Lithiation-Delithiation of SnO Anodes in Li-Ion Batteries. Physical Review Applied, 2015, 4, .	1.5	6
12	Pushing back the limit of ab-initio quantum transport simulations on hybrid supercomputers. , 2015, , .		16
13	Long-Time-Scale Simulations of H₂O Admolecule Diffusion on Ice Ih(0001) Surfaces. Journal of Physical Chemistry C, 2015, 119, 16528-16536.	1.5	15
14	Magic-Number Gold Nanoclusters with Diameters from 1 to 3.5 nm: Relative Stability and Catalytic Activity for CO Oxidation. Nano Letters, 2015, 15, 682-688.	4.5	92
15	Lithiation of Tin Oxide: A Computational Study. ACS Applied Materials & Interfaces, 2014, 6, 22257-22263.	4.0	14
16	EON: software for long time simulations of atomic scale systems. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 055002.	0.8	58
17	Molecular reordering processes on ice (0001) surfaces from long timescale simulations. Journal of Chemical Physics, 2014, 141, 234706.	1.2	17
18	Bowl breakout: Escaping the positive region when searching for saddle points. Journal of Chemical Physics, 2014, 141, 024109.	1.2	9

#	Article	IF	Citations
19	Geothermal model calibration using a global minimization algorithm based on finding saddle points and minima of the objective function. Computers and Geosciences, 2014, 65, 110-117.	2.0	22
20	Improved initial guess for minimum energy path calculations. Journal of Chemical Physics, 2014, 140, 214106.	1.2	279
21	Vacuum microdiodes as tunable THZ oscillators. , 2013, , .		0
22	Tunability of the terahertz space-charge modulation in a vacuum microdiode. Physics of Plasmas, 2013, 20, .	0.7	15
23	Stability and mobility of vacancyâ€“H complexes in Al. Journal of Physics Condensed Matter, 2013, 25, 375401.	0.7	5
24	Parametric survey of space-charge modulations in vacuum microdiodes. , 2012, , .		0
25	Long-timescale simulations of diffusion in molecular solids. Physical Chemistry Chemical Physics, 2012, 14, 10844.	1.3	22
26	Simulated Annealing with Coarse Graining and Distributed Computing. Lecture Notes in Computer Science, 2012, , 34-44.	1.0	17
27	Efficient Sampling of Saddle Points with the Minimum-Mode Following Method. SIAM Journal of Scientific Computing, 2011, 33, 633-652.	1.3	23
28	PHOTOELECTRIC CHARGING OF DUST GRAINS IN THE ENVIRONMENT OF YOUNG STELLAR OBJECTS. Astrophysical Journal, 2011, 740, 77.	1.6	13
29	Distributed implementation of the adaptive kinetic Monte Carlo method. Mathematics and Computers in Simulation, 2010, 80, 1487-1498.	2.4	17
30	Space-Charge Modulation in Vacuum Microdiodes at THz Frequencies. Physical Review Letters, 2010, 104, 175002.	2.9	56
31	Finding mechanism of transitions in complex systems: formation and migration of dislocation kinks in a silicon crystal. Journal of Physics Condensed Matter, 2009, 21, 084210.	0.7	15
32	Long time scale simulation of a grain boundary in copper. New Journal of Physics, 2009, 11, 073034.	1.2	20
33	Simulations of hydrogen diffusion at grain boundaries in aluminum. Acta Materialia, 2009, 57, 4036-4045.	3.8	78
34	Theoretical study of kinks on screw dislocation in silicon. Physical Review B, 2008, 77, .	1.1	49