Nicolas Salles

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8904617/publications.pdf

Version: 2024-02-01

13	81	1478505 6	1474206 9
papers	citations	h-index	g-index

13	13	13	102
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Atomistic simulation and interatomic potential comparison in Î±-Al₂O₃: lattice, surface and extended-defects properties. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 035008.	2.0	7
2	Iterative Rotations and Assignments (IRA): A shape matching algorithm for atomic structures. Software Impacts, 2022, 12, 100264.	1.4	2
3	Activationâ€“Relaxation Technique: An efficient way to find minima and saddle points of potential energy surfaces. Computational Materials Science, 2022, 209, 111363.	3.0	5
4	IRA: A Shape Matching Approach for Recognition and Comparison of Generic Atomic Patterns. Journal of Chemical Information and Modeling, 2021, 61, 5446-5457.	5.4	3
5	Kinetic Monte Carlo for Process Simulation: First Principles Calibrated Parameters for BO2. , 2021, , .		0
6	Improved SMTB-Q model applied to oxygen migration and pressure phase transitions in UO2. Journal of Physics Condensed Matter, 2020, 32, 095701.	1.8	3
7	Collective dipole effects in ionic transport under electric fields. Nature Communications, 2020, 11, 3330.	12.8	6
8	Finding Reaction Pathways and Transition States: r-ARTn and d-ARTn as an Efficient and Versatile Alternative to String Approaches. Journal of Chemical Theory and Computation, 2020, 16, 6726-6734.	5.3	21
9	Modeling of the interface formation during CuO deposition on Al(111) substrate: linking material design and elaboration process parameters through multi-levels approach. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 064005.	2.0	1
10	Strain-driven diffusion process during silicon oxidation investigated by coupling density functional theory and activation relaxation technique. Journal of Chemical Physics, 2017, 147, 054701.	3.0	6
11	Molecular dynamics study of high-pressure alumina polymorphs with a tight-binding variable-charge model. Computational Materials Science, 2016, 111, 181-189.	3.0	9
12	Improved Tight-Binding Charge Transfer Model and Calculations of Energetics of a Step on the Rutile TiO₂(110) Surface. Journal of Physical Chemistry C, 2015, 119, 10391-10399.	3.1	8
13	SrTiO3 (001) surface and strained thin films: Atomic simulations using a tight-binding variable-charge model. Surface Science, 2013, 616, 19-28.	1.9	10