

Nicolas Salles

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Atomistic simulation and interatomic potential comparison in γ -Al ₂ O ₃ : lattice, surface and extended-defects properties. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 035008.	0.8	7
2	Iterative Rotations and Assignments (IRA): A shape matching algorithm for atomic structures. Software Impacts, 2022, 12, 100264.	0.8	2
3	Activation-Relaxation Technique: An efficient way to find minima and saddle points of potential energy surfaces. Computational Materials Science, 2022, 209, 111363.	1.4	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.	2.5	3
5	Kinetic Monte Carlo for Process Simulation: First Principles Calibrated Parameters for BO ₂ . , 2021, , .		0
6	Improved SMTB-Q model applied to oxygen migration and pressure phase transitions in UO ₂ . Journal of Physics Condensed Matter, 2020, 32, 095701.	0.7	3
7	Collective dipole effects in ionic transport under electric fields. Nature Communications, 2020, 11, 3330.	5.8	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.	2.3	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.	0.8	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.	1.2	6
11	Molecular dynamics study of high-pressure alumina polymorphs with a tight-binding variable-charge model. Computational Materials Science, 2016, 111, 181-189.	1.4	9
12	Improved Tight-Binding Charge Transfer Model and Calculations of Energetics of a Step on the Rutile TiO ₂ (110) Surface. Journal of Physical Chemistry C, 2015, 119, 10391-10399.	1.5	8
13	SrTiO ₃ (001) surface and strained thin films: Atomic simulations using a tight-binding variable-charge model. Surface Science, 2013, 616, 19-28.	0.8	10