

# Nicolas Salles

## List of Publications by Year in descending order

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13  
papers

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1478505  
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docs citations

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times ranked

102  
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	SrTiO <sub>3</sub> (001) surface and strained thin films: Atomic simulations using a tight-binding variable-charge model. Surface Science, 2013, 616, 19-28.	1.9	10
3	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
4	Improved Tight-Binding Charge Transfer Model and Calculations of Energetics of a Step on the Rutile TiO <sub>2</sub> (110) Surface. Journal of Physical Chemistry C, 2015, 119, 10391-10399.	3.1	8
5	Atomistic simulation and interatomic potential comparison in $\gamma$ -Al <sub>2</sub> O <sub>3</sub> : lattice, surface and extended-defects properties. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 035008.	2.0	7
6	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
7	Collective dipole effects in ionic transport under electric fields. Nature Communications, 2020, 11, 3330.	12.8	6
8	Activation-Relaxation Technique: An efficient way to find minima and saddle points of potential energy surfaces. Computational Materials Science, 2022, 209, 111363.	3.0	5
9	Improved SMTB-Q model applied to oxygen migration and pressure phase transitions in UO <sub>2</sub> . Journal of Physics Condensed Matter, 2020, 32, 095701.	1.8	3
10	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
11	Iterative Rotations and Assignments (IRA): A shape matching algorithm for atomic structures. Software Impacts, 2022, 12, 100264.	1.4	2
12	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
13	Kinetic Monte Carlo for Process Simulation: First Principles Calibrated Parameters for BO <sub>2</sub> . , 2021, , .		0