TomÃ¡s A Arias

List of Publications by Year
in descending order

33 papers	12,873 citations	361045 20 h-index	395343 33 g-index
33 all docs	33 docs citations	33 times ranked	11388 citing authors

#	Article	IF	Citations
1	Iterative minimization techniques forab initiototal-energy calculations: molecular dynamics and conjugate gradients. Reviews of Modern Physics, 1992, 64, 1045-1097.	16.4	8,643
2	Implicit solvation model for density-functional study of nanocrystal surfaces and reaction pathways. Journal of Chemical Physics, 2014, 140, 084106.	1.2	1,676
3	Electronâ^'Phonon Scattering in Metallic Single-Walled Carbon Nanotubes. Nano Letters, 2004, 4, 517-520.	4.5	676
4	Designing solid-liquid interphases for sodium batteries. Nature Communications, 2017, 8, 898.	5.8	303
5	JDFTx: Software for joint density-functional theory. SoftwareX, 2017, 6, 278-284.	1.2	238
6	Grand canonical electronic density-functional theory: Algorithms and applications to electrochemistry. Journal of Chemical Physics, 2017, 146, 114104.	1.2	211
7	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies. Chemical Reviews, 2022, 122, 6117-6321.	23.0	195
8	Ab InitioStudy of Screw Dislocations in Mo and Ta: A New Picture of Plasticity in bcc Transition Metals. Physical Review Letters, 2000, 84, 1499-1502.	2.9	185
9	Elastic effects of vacancies in strontium titanate: Short- and long-range strain fields, elastic dipole tensors, and chemical strain. Physical Review B, 2009, 80, .	1.1	117
10	Direct visualization of sulfur cathodes: new insights into Liâ€“S batteries via operando X-ray based methods. Energy and Environmental Science, 2018, 11, 202-210.	15.6	96
11	Structure of the Photo-catalytically Active Surface of SrTiO₃. Journal of the American Chemical Society, 2016, 138, 7816-7819.	6.6	64
12	Micrometer-sized electrically programmable shape-memory actuators for low-power microrobotics. Science Robotics, 2021, 6, .	9.9	62
13	Improved tensor-product expansions for the two-particle density matrix. Physical Review A, 2002, 65, .	1.0	59
14	Spicing up continuum solvation models with SaLSA: The spherically averaged liquid susceptibility ansatz. Journal of Chemical Physics, 2015, 142, 054102.	1.2	48
15	AbÂInitio Mismatched Interface Theory of Graphene on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mrow><mml:mi>RuCl</mml:mi> : Doping and Magnetism. Physical Review Letters, 2020, 124, 106804.	2.9	39
16	Ultracold Electrons via Near-Threshold Photoemission from Single-Crystal Cu(100). Physical Review Letters, 2020, 125, 054801.	2.9	35
17	Three-Dimensional Imaging of Carbon Nanotubes Deformed by Metal Islands. Nano Letters, 2007, 7, 3770-3773.	4.5	31
18	Weighted-density functionals for cavity formation and dispersion energies in continuum solvation models. Journal of Chemical Physics, 2014, 141, 134105.	1.2	26

#	Article	IF	Citations
19	A recipe for free-energy functionals of polarizable molecular fluids. Journal of Chemical Physics, 2014, 140, 144504.	1.2	24
20	Atomic-level physics of grain boundaries in bcc molybdenum. Physical Review B, 2001, 64, .	1.1	22
21	Multiresolution analysis for efficient, high precision all-electron density-functional calculations. Physical Review B, 2002, 65, .	1.1	20
22	Density-functional fluctuation theory of crowds. Nature Communications, 2018, 9, 3538.	5.8	20
23	Single-Crystal Alkali Antimonide Photocathodes: High Efficiency in the Ultrathin Limit. Physical Review Letters, 2022, 128, 114801.	2.9	20
24	Analysis of magnetic vortex dissipation in Sn-segregated boundaries in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Nb</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math> superconducting RF cavities. Physical Review B, 2021, 103, .	1.1	12
25	Accurate calculations of the Peierls stress in small periodic cells. Journal of Computer-Aided Materials Design, 2001, 8, 161-172.	0.7	11
26	Effect of the density of states at the Fermi level on defect free energies and superconductivity: A case study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Nb</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2021, 103, .	1.1	10
27	Suppression of nano-hydride growth on Nb(100) due to nitrogen doping. Journal of Chemical Physics, 2020, 152, 214703.	1.2	9
28	Ab initio theory of the impact of grain boundaries and substitutional defects on superconducting Nb₃Sn. Superconductor Science and Technology, 2021, 34, 015015.	1.8	9
29	Importance of bulk excitations and coherent electron-photon-phonon scattering in photoemission from PbTe(111): Ab initio theory with experimental comparisons. Physical Review B, 2021, 104, .	1.1	4
30	Nanoscale Imaging of Lithium Ion Distribution During In Situ Operation of a Battery Electrode and Electrolyte. Microscopy and Microanalysis, 2014, 20, 1524-1525.	0.2	2
31	Computationally efficient dielectric calculations of molecular crystals. Journal of Chemical Physics, 2015, 142, 214101.	1.2	2
32	Low energy photoemission from (100) Ba1âˆ’xLaxSnO3 thin films for photocathode applications. European Physical Journal: Special Topics, 2019, 228, 713-718.	1.2	2
33	A combined helium atom scattering and density-functional theory study of the Nb(100) surface oxide reconstruction: Phonon band structures and vibrational dynamics. Journal of Chemical Physics, 2022, 156, 124702.	1.2	2