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	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies. Chemical Reviews, 2022, 122, 6117-6321.	23.0	195
2	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
3	Single-Crystal Alkali Antimonide Photocathodes: High Efficiency in the Ultrathin Limit. Physical Review Letters, 2022, 128, 114801.	2.9	20
4	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> superconducting RF cavities. Physical Review B, 2021, 103, .	1.1	12
5	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:mn> Physical Review B, 2021, 103, .	1.1	10
6	Micrometer-sized electrically programmable shape-memory actuators for low-power microrobotics. Science Robotics, 2021, 6, .	9.9	62
7	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
8	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
9	Ultracold Electrons via Near-Threshold Photoemission from Single-Crystal Cu(100). Physical Review Letters, 2020, 125, 054801.	2.9	35
10	Suppression of nano-hydride growth on Nb(100) due to nitrogen doping. Journal of Chemical Physics, 2020, 152, 214703.	1.2	9
11	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
12	Low energy photoemission from (100) Ba1â^'xLaxSnO3 thin films for photocathode applications. European Physical Journal: Special Topics, 2019, 228, 713-718.	1.2	2
13	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
14	Density-functional fluctuation theory of crowds. Nature Communications, 2018, 9, 3538.	5.8	20
15	Grand canonical electronic density-functional theory: Algorithms and applications to electrochemistry. Journal of Chemical Physics, 2017, 146, 114104.	1.2	211
16	Designing solid-liquid interphases for sodium batteries. Nature Communications, 2017, 8, 898.	5.8	303
17	JDFTx: Software for joint density-functional theory. SoftwareX, 2017, 6, 278-284.	1.2	238
18	Structure of the Photo-catalytically Active Surface of SrTiO₃. Journal of the American Chemical Society, 2016, 138, 7816-7819.	6.6	64

#	Article	IF	Citations
19	Spicing up continuum solvation models with SaLSA: The spherically averaged liquid susceptibility ansatz. Journal of Chemical Physics, 2015, 142, 054102.	1.2	48
20	Computationally efficient dielectric calculations of molecular crystals. Journal of Chemical Physics, 2015, 142, 214101.	1.2	2
21	A recipe for free-energy functionals of polarizable molecular fluids. Journal of Chemical Physics, 2014, 140, 144504.	1.2	24
22	Implicit solvation model for density-functional study of nanocrystal surfaces and reaction pathways. Journal of Chemical Physics, 2014, 140, 084106.	1.2	1,676
23	Weighted-density functionals for cavity formation and dispersion energies in continuum solvation models. Journal of Chemical Physics, 2014, 141, 134105.	1.2	26
24	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
25	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
26	Three-Dimensional Imaging of Carbon Nanotubes Deformed by Metal Islands. Nano Letters, 2007, 7, 3770-3773.	4.5	31
27	Electronâ˜Phonon Scattering in Metallic Single-Walled Carbon Nanotubes. Nano Letters, 2004, 4, 517-520.	4.5	676
28	Improved tensor-product expansions for the two-particle density matrix. Physical Review A, 2002, 65, .	1.0	59
29	Multiresolution analysis for efficient, high precision all-electron density-functional calculations. Physical Review B, 2002, 65, .	1.1	20
30	Accurate calculations of the Peierls stress in small periodic cells. Journal of Computer-Aided Materials Design, 2001, 8, 161-172.	0.7	11
31	Atomic-level physics of grain boundaries in bcc molybdenum. Physical Review B, 2001, 64, .	1.1	22
32	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
33	Iterative minimization techniques forab initiototal-energy calculations: molecular dynamics and conjugate gradients. Reviews of Modern Physics, 1992, 64, 1045-1097.	16.4	8,643