Toms A Arias

List of Publications by Year in Descending Order

33 papers	10,304 citations	19 h-index	33 g-index
33 ext. papers	11,497 ext. citations	10.1 avg, IF	5.72 L-index

#	Paper	IF	Citations
33	Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies.. *Chemical Reviews*, **2022**,	68.1	25
32	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	3.9	
31	Single-Crystal Alkali Antimonide Photocathodes: High Efficiency in the Ultrathin Limit.. *Physical Review Letters*, **2022**, 128, 114801	7.4	4
30	Ab initio theory of the impact of grain boundaries and substitutional defects on superconducting Nb3Sn. *Superconductor Science and Technology*, **2021**, 34, 015015	3.1	5
29	Effect of the density of states at the Fermi level on defect free energies and superconductivity: A case study of Nb3Sn. *Physical Review B*, **2021**, 103,	3.3	2
28	Micrometer-sized electrically programmable shape-memory actuators for low-power microrobotics. *Science Robotics*, **2021**, 6,	18.6	19
27	Analysis of magnetic vortex dissipation in Sn-segregated boundaries in Nb3Sn superconducting RF cavities. *Physical Review B*, **2021**, 103,	3.3	2
26	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,	3.3	2
25	Suppression of nano-hydride growth on Nb(100) due to nitrogen doping. *Journal of Chemical Physics*, **2020**, 152, 214703	3.9	6
24	Ab□Initio Mismatched Interface Theory of Graphene on □RuCl_{3}: Doping and Magnetism. *Physical Review Letters*, **2020**, 124, 106804	7.4	18
23	Ultracold Electrons via Near-Threshold Photoemission from Single-Crystal Cu(100). *Physical Review Letters*, **2020**, 125, 054801	7.4	13
22	Low energy photoemission from (100) Ba1□LaxSnO3 thin films for photocathode applications. *European Physical Journal: Special Topics*, **2019**, 228, 713-718	2.3	2
21	Direct visualization of sulfur cathodes: new insights into Li-S batteries via X-ray based methods.. *Energy and Environmental Science*, **2018**, 8, 202-210	35.4	67
20	Density-functional fluctuation theory of crowds. *Nature Communications*, **2018**, 9, 3538	17.4	12
19	Grand canonical electronic density-functional theory: Algorithms and applications to electrochemistry. *Journal of Chemical Physics*, **2017**, 146, 114104	3.9	117
18	Designing solid-liquid interphases for sodium batteries. *Nature Communications*, **2017**, 8, 898	17.4	212
17	JDFTx: software for joint density-functional theory. *SoftwareX*, **2017**, 6, 278-284	2.7	130

16	Structure of the Photo-catalytically Active Surface of SrTiO3. *Journal of the American Chemical Society*, **2016**, 138, 7816-9	16.4	54
15	Spicing up continuum solvation models with SaLSA: the spherically averaged liquid susceptibility ansatz. *Journal of Chemical Physics*, **2015**, 142, 054102	3.9	40
14	Computationally efficient dielectric calculations of molecular crystals. *Journal of Chemical Physics*, **2015**, 142, 214101	3.9	2
13	A recipe for free-energy functionals of polarizable molecular fluids. *Journal of Chemical Physics*, **2014**, 140, 144504	3.9	22
12	Implicit solvation model for density-functional study of nanocrystal surfaces and reaction pathways. *Journal of Chemical Physics*, **2014**, 140, 084106	3.9	945
11	Weighted-density functionals for cavity formation and dispersion energies in continuum solvation models. *Journal of Chemical Physics*, **2014**, 141, 134105	3.9	25
10	Nanoscale Imaging of Lithium Ion Distribution During In Situ Operation of a Battery Electrode and Electrolyte. *Microscopy and Microanalysis*, **2014**, 20, 1524-1525	0.5	0
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,	3.3	103
8	Three-Dimensional Imaging of Carbon Nanotubes Deformed by Metal Islands. *Nano Letters*, **2007**, 7, 3770-3773	11.5	29
7	Electron−Phonon Scattering in Metallic Single-Walled Carbon Nanotubes. *Nano Letters*, **2004**, 4, 517-520	11.5	594
6	Improved tensor-product expansions for the two-particle density matrix. *Physical Review A*, **2002**, 65,	2.6	54
5	Multiresolution analysis for efficient, high precision all-electron density-functional calculations. *Physical Review B*, **2002**, 65,	3.3	19
4	Accurate calculations of the Peierls stress in small periodic cells. *Journal of Computer-Aided Materials Design*, **2001**, 8, 161-172		11
3	Atomic-level physics of grain boundaries in bcc molybdenum. *Physical Review B*, **2001**, 64,	3.3	22
2	Ab initio study of screw dislocations in Mo and ta: A new picture of plasticity in bcc transition metals. *Physical Review Letters*, **2000**, 84, 1499-502	7.4	172
1	Iterative minimization techniques for ab initio total-energy calculations: molecular dynamics and conjugate gradients. *Reviews of Modern Physics*, **1992**, 64, 1045-1097	40.5	7576