# Toms A Arias

## List of Publications by Citations



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|---|---|---|---|
| 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 | 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 |
| 32 | Implicit solvation model for density-functional study of nanocrystal surfaces and reaction pathways. *Journal of Chemical Physics*, **2014**, 140, 084106 | 3.9 | 945 |
| 31 | Electron-Phonon Scattering in Metallic Single-Walled Carbon Nanotubes. *Nano Letters*, **2004**, 4, 517-520 | 11.5 | 594 |
| 30 | Designing solid-liquid interphases for sodium batteries. *Nature Communications*, **2017**, 8, 898 | 17.4 | 212 |
| 29 | 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 |
| 28 | JDFTx: software for joint density-functional theory. *SoftwareX*, **2017**, 6, 278-284 | 2.7 | 130 |
| 27 | Grand canonical electronic density-functional theory: Algorithms and applications to electrochemistry. *Journal of Chemical Physics*, **2017**, 146, 114104 | 3.9 | 117 |
| 26 | 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 |
| 25 | 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 |
| 24 | Structure of the Photo-catalytically Active Surface of SrTiO3. *Journal of the American Chemical Society*, **2016**, 138, 7816-9 | 16.4 | 54 |
| 23 | Improved tensor-product expansions for the two-particle density matrix. *Physical Review A*, **2002**, 65, | 2.6 | 54 |
| 22 | Spicing up continuum solvation models with SaLSA: the spherically averaged liquid susceptibility ansatz. *Journal of Chemical Physics*, **2015**, 142, 054102 | 3.9 | 40 |
| 21 | Three-Dimensional Imaging of Carbon Nanotubes Deformed by Metal Islands. *Nano Letters*, **2007**, 7, 3770-3773 | 11.5 | 29 |
| 20 | Weighted-density functionals for cavity formation and dispersion energies in continuum solvation models. *Journal of Chemical Physics*, **2014**, 141, 134105 | 3.9 | 25 |
| 19 | Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies.. *Chemical Reviews*, **2022**, | 68.1 | 25 |
| 18 | A recipe for free-energy functionals of polarizable molecular fluids. *Journal of Chemical Physics*, **2014**, 140, 144504 | 3.9 | 22 |
| 17 | Atomic-level physics of grain boundaries in bcc molybdenum. *Physical Review B*, **2001**, 64, | 3.3 | 22 |

# List of Publications

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|---|---|---|---|
| 16 | Multiresolution analysis for efficient, high precision all-electron density-functional calculations. *Physical Review B*, **2002**, 65, | 3.3 | 19 |
| 15 | Micrometer-sized electrically programmable shape-memory actuators for low-power microrobotics. *Science Robotics*, **2021**, 6, | 18.6 | 19 |
| 14 | Ab□Initio Mismatched Interface Theory of Graphene on □RuCl_{3}: Doping and Magnetism. *Physical Review Letters*, **2020**, 124, 106804 | 7.4 | 18 |
| 13 | Ultracold Electrons via Near-Threshold Photoemission from Single-Crystal Cu(100). *Physical Review Letters*, **2020**, 125, 054801 | 7.4 | 13 |
| 12 | Density-functional fluctuation theory of crowds. *Nature Communications*, **2018**, 9, 3538 | 17.4 | 12 |
| 11 | Accurate calculations of the Peierls stress in small periodic cells. *Journal of Computer-Aided Materials Design*, **2001**, 8, 161-172 | | 11 |
| 10 | Suppression of nano-hydride growth on Nb(100) due to nitrogen doping. *Journal of Chemical Physics*, **2020**, 152, 214703 | 3.9 | 6 |
| 9 | 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 |
| 8 | Single-Crystal Alkali Antimonide Photocathodes: High Efficiency in the Ultrathin Limit.. *Physical Review Letters*, **2022**, 128, 114801 | 7.4 | 4 |
| 7 | Computationally efficient dielectric calculations of molecular crystals. *Journal of Chemical Physics*, **2015**, 142, 214101 | 3.9 | 2 |
| 6 | Low energy photoemission from (100) Ba1□LaxSnO3 thin films for photocathode applications. *European Physical Journal: Special Topics*, **2019**, 228, 713-718 | 2.3 | 2 |
| 5 | 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 |
| 4 | Analysis of magnetic vortex dissipation in Sn-segregated boundaries in Nb3Sn superconducting RF cavities. *Physical Review B*, **2021**, 103, | 3.3 | 2 |
| 3 | 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 |
| 2 | 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 |
| 1 | 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 | |