Leonardo Medrano Sandonas

List of Publications by Year
in descending order

28 papers	491 citations	758635 12 h-index	676716 22 g-index
30 all docs	30 docs citations	30 times ranked	740 citing authors

#	Article	IF	Citations
1	Anisotropic Thermoelectric Response in Two-Dimensional Puckered Structures. Journal of Physical Chemistry C, 2016, 120, 18841-18849.	1.5	84
2	Accurate Many-Body Repulsive Potentials for Density-Functional Tight Binding from Deep Tensor Neural Networks. Journal of Physical Chemistry Letters, 2020, 11, 6835-6843.	2.1	55
3	QM7-X, a comprehensive dataset of quantum-mechanical properties spanning the chemical space of small organic molecules. Scientific Data, 2021, 8, 43.	2.4	46
4	Thermal bridging of graphene nanosheets via covalent molecular junctions: A non-equilibrium Greenâ€™s functionsâ€“density functional tight-binding study. Nano Research, 2019, 12, 791-799.	5.8	29
5	Enhancement of thermal transport properties of asymmetric Graphene/hBN nanoribbon heterojunctions by substrate engineering. Carbon, 2017, 124, 642-650.	5.4	27
6	In-Situ Stretching Patterned Graphene Nanoribbons in the Transmission Electron Microscope. Scientific Reports, 2017, 7, 211.	1.6	26
7	Copper Induced Conformational Changes of Tripeptide Monolayer Based Impedimetric Biosensor. Scientific Reports, 2017, 7, 9498.	1.6	20
8	Polymerization driven monomer passage through monolayer chemical vapour deposition graphene. Nature Communications, 2018, 9, 4051.	5.8	20
9	Tuning quantum electron and phonon transport in two-dimensional materials by strain engineering: a Green's function based study. Physical Chemistry Chemical Physics, 2017, 19, 1487-1495.	1.3	19
10	Firstâ€Principleâ€Based Phonon Transport Properties of Nanoscale Graphene Grain Boundaries. Advanced Science, 2018, 5, 1700365.	5.6	17
11	Engineering thermal rectification in MoS₂nanoribbons: a non-equilibrium molecular dynamics study. RSC Advances, 2015, 5, 54345-54351.	1.7	16
12	Green function, quasi-classical Langevin and Kuboâ€“Greenwood methods in quantum thermal transport. Journal of Physics Condensed Matter, 2019, 31, 273003.	0.7	15
13	Electron Transport through Self-Assembled Monolayers of Tripeptides. Journal of Physical Chemistry C, 2019, 123, 9600-9608.	1.5	13
14	Thermoelectric properties of functionalized graphene grain boundaries. Journal of Self-Assembly and Molecular Electronics (SAME), 2015, 2015, 1-20.	0.0	13
15	Quantum Phonon Transport in Nanomaterials: Combining Atomistic with Non-Equilibrium Greenâ€™s Function Techniques. Entropy, 2019, 21, 735.	1.1	12
16	Determination of the threshold of nanoparticle behavior: Structural and electronic properties study of nano-sized copper. Physica B: Condensed Matter, 2014, 436, 74-79.	1.3	11
17	Molecular and Ionic Dipole Effects on the Electronic Properties of Si-/SiO₂-Grafted Alkylamine Monolayers. ACS Applied Materials & Interfaces, 2017, 9, 44873-44879.	4.0	10
18	Doping engineering of thermoelectric transport in BNC heteronanotubes. Physical Chemistry Chemical Physics, 2019, 21, 1904-1911.	1.3	10

#	Article	IF	Citations
19	Influence of chemical disorder on the electronic level spacing distribution of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si0010.gif" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Ag</mml:mi></mml:mrow><mml:mrow><mml:mn>5083</mml:mn></mml:mrow> nanoparticle: A tight-binding study. Physica B: Condensed Matter, 2013, 412, 122-125.	1.3	7
20	Structural distortions in molecular-based quantum cellular automata: a minimal model based study. Physical Chemistry Chemical Physics, 2014, 16, 17777-17785.	1.3	7
21	Implementation of an alternative method to determine the critical cooling rate: Application in silver and copper nanoparticles. Chemical Physics Letters, 2014, 612, 273-279.	1.2	7
22	Impact of device geometry on electron and phonon transport in graphene nanorings. Physical Review B, 2019, 99, .	1.1	7
23	Selective Transmission of Phonons in Molecular Junctions with Nanoscopic Thermal Baths. Journal of Physical Chemistry C, 2019, 123, 9680-9687.	1.5	7
24	An Atomistic Study of the Thermoelectric Signatures of CNT Peapods. Journal of Physical Chemistry C, 2021, 125, 13721-13731.	1.5	5
25	Atomistic Framework for Time-Dependent Thermal Transport. Journal of Physical Chemistry C, 2018, 122, 21062-21068.	1.5	3
26	Disorder-induced metal-insulator transition in cooled silver and copper nanoparticles: A statistical study. Chemical Physics Letters, 2017, 681, 22-28.	1.2	2
27	Exploring the write-in process in molecular quantum cellular automata: a combined modelingand first-principle approach. Journal of Physics Condensed Matter, 2019, 31, 405502.	0.7	1
28	Nanoscale Phononic Analog of the Ranque-Hilsch Vortex Tube. Physical Review Applied, 2021, 15, .	1.5	1