Leonardo Medrano Sandonas

List of Publications by Year
in descending order

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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	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
2	Nanoscale Phononic Analog of the Ranque-Hilsch Vortex Tube. Physical Review Applied, 2021, 15, .	1.5	1
3	An Atomistic Study of the Thermoelectric Signatures of CNT Peapods. Journal of Physical Chemistry C, 2021, 125, 13721-13731.	1.5	5
4	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
5	Green function, quasi-classical Langevin and Kuboâ€“Greenwood methods in quantum thermal transport. Journal of Physics Condensed Matter, 2019, 31, 273003.	0.7	15
6	Quantum Phonon Transport in Nanomaterials: Combining Atomistic with Non-Equilibrium Greenâ€™s Function Techniques. Entropy, 2019, 21, 735.	1.1	12
7	Doping engineering of thermoelectric transport in BNC heteronanotubes. Physical Chemistry Chemical Physics, 2019, 21, 1904-1911.	1.3	10
8	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
9	Impact of device geometry on electron and phonon transport in graphene nanorings. Physical Review B, 2019, 99, .	1.1	7
10	Electron Transport through Self-Assembled Monolayers of Tripeptides. Journal of Physical Chemistry C, 2019, 123, 9600-9608.	1.5	13
11	Selective Transmission of Phonons in Molecular Junctions with Nanoscopic Thermal Baths. Journal of Physical Chemistry C, 2019, 123, 9680-9687.	1.5	7
12	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
13	Firstâ€Principleâ€Based Phonon Transport Properties of Nanoscale Graphene Grain Boundaries. Advanced Science, 2018, 5, 1700365.	5.6	17
14	Polymerization driven monomer passage through monolayer chemical vapour deposition graphene. Nature Communications, 2018, 9, 4051.	5.8	20
15	Atomistic Framework for Time-Dependent Thermal Transport. Journal of Physical Chemistry C, 2018, 122, 21062-21068.	1.5	3
16	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
17	Disorder-induced metal-insulator transition in cooled silver and copper nanoparticles: A statistical study. Chemical Physics Letters, 2017, 681, 22-28.	1.2	2
18	Enhancement of thermal transport properties of asymmetric Graphene/hBN nanoribbon heterojunctions by substrate engineering. Carbon, 2017, 124, 642-650.	5.4	27

#	Article	IF	Citations
19	Copper Induced Conformational Changes of Tripeptide Monolayer Based Impedimetric Biosensor. Scientific Reports, 2017, 7, 9498.	1.6	20
20	In-Situ Stretching Patterned Graphene Nanoribbons in the Transmission Electron Microscope. Scientific Reports, 2017, 7, 211.	1.6	26
21	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
22	Anisotropic Thermoelectric Response in Two-Dimensional Puckered Structures. Journal of Physical Chemistry C, 2016, 120, 18841-18849.	1.5	84
23	Engineering thermal rectification in MoS₂nanoribbons: a non-equilibrium molecular dynamics study. RSC Advances, 2015, 5, 54345-54351.	1.7	16
24	Thermoelectric properties of functionalized graphene grain boundaries. Journal of Self-Assembly and Molecular Electronics (SAME), 2015, 2015, 1-20.	0.0	13
25	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
26	Structural distortions in molecular-based quantum cellular automata: a minimal model based study. Physical Chemistry Chemical Physics, 2014, 16, 17777-17785.	1.3	7
27	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
28	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