Matheus P Lima

List of Publications by Year
in descending order

38	555	623734 14	677142 22
papers	citations	h-index	g-index

38	38	38	681
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Edge effects in bilayer graphene nanoribbons:Ab initiototal-energy density functional theory calculations. Physical Review B, 2009, 79, .	3.2	58
2	Dynamical evolution of polaron to bipolaron in conjugated polymers. Physical Review B, 2006, 74, .	3.2	53
3	Bilayer graphene dual-gate nanodevice: Anab initiosimulation. Physical Review B, 2011, 84, .	3.2	36
4	Adatoms in graphene as a source of current polarization: Role of the local magnetic moment. Physical Review B, 2011, 84, .	3.2	27
5	First-Principles Exploration of Two-Dimensional Transition Metal Dichalcogenides Based on Fe, Co, Ni, and Cu Groups and Their van der Waals Heterostructures. ACS Applied Energy Materials, 2019, 2, 8491-8501.	5.1	27
6	Role of Structural Phases and Octahedra Distortions in the Optoelectronic and Excitonic Properties of CsGeX₃ (X = Cl, Br, I) Perovskites. Journal of Physical Chemistry C, 2021, 125, 19142-19155.	3.1	26
7	Topological phases in triangular lattices of Ru adsorbed on graphene:Ab initiocalculations. Physical Review B, 2014, 89, .	3.2	25
8	Ab Initio Investigation of Atomistic Insights into the Nanoflake Formation of Transition-Metal Dichalcogenides: The Examples of MoS₂, MoSe₂, and MoTe₂. Journal of Physical Chemistry C, 2018, 122, 27059-27069.	3.1	24
9	Edge, size, and shape effects on WS₂, WSe₂, and WTe₂ nanoflake stability: design principles from an ab initio investigation. Physical Chemistry Chemical Physics, 2019, 21, 23076-23084.	2.8	19
10	Tailoring the physical and chemical properties of Sn_{1â”x}Co_xO₂ nanoparticles: an experimental and theoretical approach. Physical Chemistry Chemical Physics, 2020, 22, 3702-3714.	2.8	19
11	Spin caloritronics in graphene with Mn. Applied Physics Letters, 2014, 104, .	3.3	18
12	Tuning the Magnetic Properties of FeCo Thin Films through the Magnetoelastic Effect Induced by the Au Underlayer Thickness. ACS Applied Materials & Interfaces, 2019, 11, 1529-1537.	8.0	18
13	Size-Induced Phase Evolution of MoSe₂ Nanoflakes Revealed by Density Functional Theory. Journal of Physical Chemistry C, 2018, 122, 20483-20488.	3.1	17
14	Azobenzene Adsorption on the MoS₂(0001) Surface: A Density Functional Investigation within van der Waals Corrections. Journal of Physical Chemistry C, 2018, 122, 18895-18901.	3.1	15
15	Insights into the nature of optically active defects of ZnO. Journal of Luminescence, 2020, 227, 117536.	3.1	15
16	Splitting of the zero-energy edge states in bilayer graphene. Physical Review B, 2010, 81, .	3.2	14
17	Effects of Side-Chain and Electron Exchange Correlation on the Band Structure of Perylene Diimide Liquid Crystals: A Density Functional Study. Journal of Physical Chemistry B, 2009, 113, 5376-5380.	2.6	12
18	Interfaces between buckling phases in silicene:Ab initiodensity functional theory calculations. Physical Review B, 2013, 88, .	3.2	11

#	Article	IF	Citations
19	Valley Hall effect in silicene and hydrogenated silicene ruled by grain boundaries: Anab initioinvestigation. Physical Review B, 2015, 91, .	3.2	11
20	Electronic transport properties of MoS2 nanoribbons embedded in butadiene solvent. Physical Chemistry Chemical Physics, 2019, 21, 11359-11366.	2.8	11
21	Stacking-dependent transport properties in few-layers graphene. Solid State Communications, 2017, 250, 70-74.	1.9	10
22	Tight-binding model for the band dispersion in rhombohedral topological insulators over the whole Brillouin zone. Physical Review B, 2018, 98, .	3.2	10
23	Silicene-Based FET for Logical Technology. IEEE Electron Device Letters, 2018, 39, 1258-1261.	3.9	10
24	Simple implementation of complex functionals: Scaled self-consistency. Journal of Chemical Physics, 2007, 126, 144107.	3.0	8
25	Mimicking nanoribbon behavior using a graphene layer on SiC. Physical Review B, 2010, 82, .	3.2	8
26	First-principles investigation of the role of Cr in the electronic properties of the two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Mo</mml:mi><mml:mi>2</mml:mi></mml:msub></mml:m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:m. Physical Review Materials, 2022, 6, .	2.4	6
27	Polaron stability under collision with different defects in conjugated polymers. International Journal of Quantum Chemistry, 2006, 106, 2603-2608.	2.0	5
28	Interplay between structure asymmetry, defect-induced localization, and spin-orbit interaction in Mn-doped quantum dots. Physical Review B, 2017, 95, .	3.2	5
29	Double-walled silicon nanotubes: anab initioinvestigation. Nanotechnology, 2018, 29, 075703.	2.6	5
30	Defect-induced magnetism in II-VI quantum dots. Physical Review B, 2019, 99, .	3.2	5
31	Tuning the magnetic properties of Sn_{1â^'xâ^'y}Ce_{4+x}Ce_{3+y}O₂ nanoparticles: an experimental and theoretical approach. Nanoscale Advances, 2021, 3, 1484-1495.	4.6	5
32	Transition of polaron to bipolaron structure in conjugated polymers. Computational and Theoretical Chemistry, 2008, 852, 15-21.	1.5	4
33	Photomodulation of transport in monolayer dichalcogenides. Physical Review B, 2018, 98, .	3.2	4
34	Polaron dynamics with impurities in conjugated polymers. Brazilian Journal of Physics, 2005, 35, 961-964.	1.4	3
35	Effects of impurities on polaron dynamics in conjugated polymers: Effective potentials. International Journal of Quantum Chemistry, 2006, 106, 2597-2602.	2.0	3
36	The role played by the molecular geometry on the electronic transport through nanometric organic films. Physical Chemistry Chemical Physics, 2019, 21, 24584-24591.	2.8	3

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37	Spatial anisotropy of the quantum spin liquid system YbMgGaO4 revealed by ab initio calculations. Journal of Physics Condensed Matter, 2020, 32, 025505.	1.8	3
38	Ab initio investigation of topological phase transitions induced by pressure in trilayer van der Waals structures: the example of h-BN/SnTe/h-BN. Journal of Physics Condensed Matter, 2021, 33, 025003.	1.8	2