Lara K Teles

List of Publications by Year
in descending order

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83 papers	2,789 citations	218592 26 h-index	175177 52 g-index
83 all docs	83 docs citations	83 times ranked	2864 citing authors

#	Article	IF	Citations
1	DFT-1/2 method applied to 2D topological insulators: fluorinated and hydrogenated group-IV honeycomb systems. Journal of Physics Condensed Matter, 2021, 33, 435501.	0.7	3
2	Atomistic Origins of Enhanced Band Gap, Miscibility, and Oxidation Resistance in Î±-CsPb1â€“xSnxI3 Mixed Perovskite. Journal of Physical Chemistry C, 2020, 124, 26124-26133.	1.5	12
3	Electronic Structure Panorama of Halide Perovskites: Approximated DFT-1/2 Quasiparticle and Relativistic Corrections. Journal of Physical Chemistry C, 2020, 124, 18390-18400.	1.5	27
4	Efficient calculation of excitonic effects in solids including approximated quasiparticle energies. Journal of Physics Condensed Matter, 2020, 32, 405505.	0.7	2
5	Relativistic DFT-1/2 Calculations Combined with a Statistical Approach for Electronic and Optical Properties of Mixed Metal Hybrid Perovskites. Journal of Physical Chemistry Letters, 2019, 10, 4245-4251.	2.1	20
6	Thermodynamic Stability and Structural Insights for CH3NH3Pb1â^'xSixI3, CH3NH3Pb1â^'xGexI3, and CH3NH3Pb1â^'xSnxI3 Hybrid Perovskite Alloys: A Statistical Approach from First Principles Calculations. Scientific Reports, 2019, 9, 11061.	1.6	14
7	Rigorous statistical thermodynamical model for lattice dynamics in alloys. Physical Review B, 2019, 100, .	1.1	3
8	Charge qubit in van der Waals heterostructures. Physical Review B, 2019, 100, .	1.1	15
9	Out-of-plane excitons in two-dimensional crystals. Physical Review B, 2019, 99, .	1.1	30
10	Quantization of spin Hall conductivity in two-dimensional topological insulators versus symmetry and spin-orbit interaction. Physical Review B, 2019, 100, .	1.1	25
11	Trends on band alignments: Validity of Anderson's rule in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SnS</mml:mi><mml:mn>2</mml:mn></mml:msub></m and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SnSe</mml:mi><mml:mn>2</mml:mn></mml:msub></ van der Waals heterostructures. Physical Review B, 2018, 97, .	1.1	57
12	Approximate quasiparticle correction for calculations of the energy gap in two-dimensional materials. Physical Review B, 2018, 97, .	1.1	20
13	Electronic properties of fluorides by efficient approximated quasiparticle DFT-1/2 and PSIC methods: BaF₂, CaF₂and CdF₂as test cases. Journal of Physics Condensed Matter, 2018, 30, 365501.	0.7	16
14	Supporting the Development of Complete Engineers. , 2018, , .		0
15	Tuning Electronic Properties and Band Alignments of Phosphorene Combined With MoSe₂ and WSe₂. Journal of Physical Chemistry C, 2017, 121, 3862-3869.	1.5	55
16	Fast and accurate approximate quasiparticle band structure calculations of ZnO, CdO, and MgO polymorphs. Physical Review B, 2017, 95, .	1.1	23
17	Optical absorbance and band-gap engineering of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mi>BN</ alloys: Phase s. Physical Review B, 2017, 95, .	1.1	24
18	General procedure for the calculation of accurate defect excitation energies from DFT-1/2 band structures: The case of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>NV</mml:mi></mml:mrow><mml:mo>â^'</m center in diamond. Physical Review B, 2017, 96, .	1.1	19

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19	Deposition of topological silicene, germanene and stanene on graphene-covered SiC substrates. Scientific Reports, 2017, 7, 15700.	1.6	36
20	Chemically Tunable Properties of Graphene Covered Simultaneously with Hydroxyl and Epoxy Groups. Journal of Physical Chemistry C, 2017, 121, 27603-27611.	1.5	6
21	Thermodynamic, electronic, and optical properties of graphene oxide: A statisticalab initioapproach. Physical Review B, 2017, 95, .	1.1	16
22	Coincidence Lattices and Interlayer Twist in van der Waals Heterostructures: Application of the Coincidence Lattice Method on $$hbox {hBN/MoSe}_2$$ hBN/MoSe 2 Heterobilayer Systems. Journal of Electronic Materials, 2017, 46, 3910-3916.	1.0	9
23	INCENTIVE ACTIONS FOR GIRLS AGED 11 TO 17 AT STEM: A BRAZILIAN CASE. , 2017, , .		0
24	First-principles determination of band-to-band electronic transition energies in cubic and hexagonal AlGaInN alloys. AIP Advances, 2016, 6, 085308.	0.6	4
25	Quantum spin Hall phase in stanene-derived overlayers on passivated SiC substrates. Physical Review B, 2016, 94, .	1.1	18
26	Influence of the composition fluctuations and decomposition on the tunable direct gap and oscillator strength of Ge1-xSnx alloys. Applied Physics Letters, 2016, 108, 092101.	1.5	19
27	Coincidence Lattices of 2D Crystals: Heterostructure Predictions and Applications. Journal of Physical Chemistry C, 2016, 120, 10895-10908.	1.5	68
28	Ab initio predictions of the stability and structural properties of zincblende (III,TM)V magnetic semiconductor alloys. Journal of Magnetism and Magnetic Materials, 2016, 405, 274-281.	1.0	4
29	Influence of structure and thermodynamic stability on electronic properties of two-dimensional SiC, SiGe, and GeC alloys. Physical Review B, 2015, 92, .	1.1	53
30	Comparing LDA-1/2, HSE03, HSE06 andG₀W₀approaches for band gap calculations of alloys. Journal of Physics Condensed Matter, 2015, 27, 505502.	0.7	45
31	Stability and electronic structure of two-dimensional allotropes of group-IV materials. Physical Review B, 2015, 92, .	1.1	124
32	Charge transition levels of Mn-doped Si calculated with the GGA-1/2 method. Physical Review B, 2014, 90, .	1.1	10
33	Theoretical study of the indium incorporation into III-V compounds revisited: The role of indium segregation and desorption. Journal of Applied Physics, 2013, 113, 033515.	1.1	8
34	Combined LDA and LDA-1/2 method to obtain defect formation energies in large silicon supercells. Physical Review B, 2013, 88, .	1.1	22
35	The LDA-1/2 technique: Recent developments. AIP Conference Proceedings, 2013, , .	0.3	8
36	All-out band structure and band offset ab initio predictions for AlN/GaN and AlP/GaP interfaces. Journal of Applied Physics, 2013, 114, .	1.1	11

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37	Digital magnetic heterostructures based on GaN using GGA-1/2 approach. Applied Physics Letters, 2012, 101, .	1.5	18
38	GaMnAs: Position of Mn-d levels and majority spin band gap predicted from GGA-1/2 calculations. Applied Physics Letters, 2012, 100, .	1.5	26
39	Slater half-occupation technique revisited: the LDA-1/2 and GGA-1/2 approaches for atomic ionization energies and band gaps in semiconductors. AIP Advances, 2011, 1, .	0.6	215
40	Accurate band gaps of AlGaN, InGaN, and AlInN alloys calculations based on LDA-1/2 approach. Applied Physics Letters, 2011, 98, .	1.5	141
41	Biaxial strain-induced suppression of spinodal decomposition in GaMnAs and GaCrAs. Journal of Applied Physics, 2010, 107, 123904.	1.1	4
42	Spin Transistors vs. Conventional Transistors: WhatÂAreÂtheÂBenefits?. Journal of Superconductivity and Novel Magnetism, 2010, 23, 61-64.	0.8	2
43	Antiferromagnetism with spin polarization of GaN-based diluted magnetic semiconductors. Physical Review B, 2010, 81, .	1.1	22
44	Simulation of a spintronic transistor: A study of its performance. Journal of Magnetism and Magnetic Materials, 2009, 321, 984-989.	1.0	8
45	Anomalous lattice parameter of magnetic semiconductor alloys. Applied Physics Letters, 2009, 94, .	1.5	15
46	Approximation to density functional theory for the calculation of band gaps of semiconductors. Physical Review B, 2008, 78, .	1.1	381
47	Influence of miscibility on the energy-gap dispersion inAlxGa1â^'xNalloys: First-principles calculations. Physical Review B, 2007, 75, .	1.1	23
48	Ab initio study of GaN/MnxGa1â^'xN digital heterostructure. AIP Conference Proceedings, 2007, , .	0.3	0
49	Theoretical support for the smaller band gap bowing in wurtzite InGaN alloys. AIP Conference Proceedings, 2007, , .	0.3	1
50	Theoretical Study of Magnetic Properties of VN, CrN, MnN, FeN and CoN under strain. AIP Conference Proceedings, 2007, , .	0.3	0
51	Energy gap and bond lengths of AlxGayIn1â€“x â€“yN, AlxGayIn1â€“x â€“yP and AlxGayIn1â€“x â€“yAs quaternary alloys. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 229-233.	0.8	0
52	Cluster expansion failings when applied to semiconductor superlattices. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 427-429.	0.8	1
53	Magnetic and electronic properties of transition metal nitride strained layers. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 269-271.	0.8	0
54	Statistical model applied toAxByC1â^'xâ^'yDquaternary alloys: Bond lengths and energy gaps ofAlxGayIn1â^'xâ^'yX(X=As, P, or N) systems. Physical Review B, 2006, 73, .	1.1	16

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55	Phase stability, chemical bonds, and gap bowing ofInxGa1â^'xNalloys: Comparison between cubic and wurtzite structures. Physical Review B, 2006, 74, .	1.1	61
56	Magnetic properties ofGaNâ•MnxGa1â^'xNdigital heterostructures: First-principles and Monte Carlo calculations. Physical Review B, 2006, 73, .	1.1	15
57	Publisher's Note:Ga1â^'xAlxNsystem, Madelung, and strain energies: A study on the quality of cluster expansions [Phys. Rev. B74, 075324 (2006)]. Physical Review B, 2006, 74, .	1.1	0
58	Theoretical prediction of ferromagnetic MnN layers embedded in wurtzite GaN. Applied Physics Letters, 2006, 88, 022507.	1.5	6
59	Ga1â^'xAlxNsystem, Madelung, and strain energies: A study on the quality of cluster expansions. Physical Review B, 2006, 74, .	1.1	5
60	Ab initio studies of indium separated phases in AlGaInN quaternary alloys. Physica Status Solidi C: Current Topics in Solid State Physics, 2005, 2, 2508-2511.	0.8	1
61	Monte Carlo simulations applied toAlxGayIn1â^'xâ^'yXquaternary alloys(X=As,P,N): A comparative study. Physical Review B, 2005, 71, .	1.1	4
62	Magnetic properties of MnN: Influence of strain and crystal structure. Applied Physics Letters, 2005, 86, 164105.	1.5	28
63	Phase separation and ordering in group-III nitride alloys. Brazilian Journal of Physics, 2004, 34, 593-597.	0.7	12
64	Microscopic description of the phase separation process inAlxGayIn1â^'xâ^'yNquaternary alloys. Physical Review B, 2004, 70, .	1.1	31
65	Theoretical study of strain-induced ordering in cubicInxGa1â^'xNepitaxial layers. Physical Review B, 2004, 69, .	1.1	13
66	Phase separation, effects of biaxial strain, and ordered phase formations in cubic nitride alloys. Microelectronics Journal, 2004, 35, 53-57.	1.1	4
67	Energy gap and optical properties of InxGa1xN. Physica Status Solidi A, 2003, 195, 628-633.	1.7	92
68	Lattice parameter and energy band gap of cubic AlxGayIn1â^'xâ^'yN quaternary alloys. Applied Physics Letters, 2003, 83, 890-892.	1.5	69
69	Full-relativistic calculations of the SrTiO3 carrier effective masses and complex dielectric function. Applied Physics Letters, 2003, 82, 3074-3076.	1.5	53
70	Strain-induced ordering in InxGa1â^'xN alloys. Applied Physics Letters, 2003, 82, 4274-4276.	1.5	13
71	Spinodal decomposition in BxGa1â^'xN and BxAl1â^'xN alloys. Applied Physics Letters, 2002, 80, 1177-1179.	1.5	41
72	Phase diagram, chemical bonds, and gap bowing of cubic InxAl1â^'xN alloys:Abâ€‰initiocalculations. Journal of Applied Physics, 2002, 92, 7109-7113.	1.1	32

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73	Phase Separation, Gap Bowing, and Structural Properties of Cubic InxAl1â€”xN. Physica Status Solidi (B): Basic Research, 2002, 234, 956-960.	0.7	12
74	Phase separation and gap bowing in zinc-blende InGaN, InAlN, BGaN, and BAlN alloy layers. Physica E: Low-Dimensional Systems and Nanostructures, 2002, 13, 1086-1089.	1.3	38
75	Phase separation suppression in InGaN epitaxial layers due to biaxial strain. Applied Physics Letters, 2002, 80, 769-771.	1.5	102
76	Structural, electronic, and effective-mass properties of silicon and zinc-blende group-III nitride semiconductor compounds. Physical Review B, 2001, 63, .	1.1	128
77	Influence of composition fluctuations and strain on gap bowing inInxGa1âˆ’xN. Physical Review B, 2001, 63, .	1.1	35
78	First-principles calculations of the thermodynamic and structural properties of strainedInxGa1âˆ’xNandAlxGa1âˆ’xNalloys. Physical Review B, 2000, 62, 2475-2485.	1.1	187
79	Relaxation Effects on the Negatively Charged Mg Impurity in Zincblende GaN. Physica Status Solidi (B): Basic Research, 1999, 216, 541-545.	0.7	6
80	Structural properties and Raman modes of zinc blende InN epitaxial layers. Applied Physics Letters, 1999, 74, 362-364.	1.5	91
81	Structural properties of cubic GaN epitaxial layers grown on Î²â€“SiC. Journal of Applied Physics, 1996, 80, 6322-6328.	1.1	8
82	Tunable Band Gap and Rhombohedral Distortion in Lead-Free CsSn1â€“xGexI3 Mixed Perovskites. Journal of Physical Chemistry C, 0, , .	1.5	3
83	Accurate and efficient approximate quasiparticle DFTâ€1/2 band structure calculations of transition metal oxide perovskites. Physica Status Solidi (B): Basic Research, 0, , .	0.7	0