Rodrigo Capaz B

List of Publications by Year
in descending order

114 papers	6,404 citations	109137 35 h-index	64668 79 g-index
115 all docs	115 docs citations	115 times ranked	9431 citing authors

#	Article	IF	Citations
1	Spatially controlled graphene- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>MoSe</mml:mi></mml:mrow><mml:mn>2</mml:mn> lateral heterostructure for sensing applications: Insights from first-principles calculations. Physical Review B, 2022, 105, .	1.1	2
2	Harnessing the photonic local density of states in graphene moirÃ© superlattices. Physical Review B, 2021, 103, .	1.1	1
3	Structural Metastability and Fermi Surface Topology of SrAl₂Si₂. Inorganic Chemistry, 2021, 60, 18652-18661.	1.9	2
4	Spiroâ€Carbon: A Metallic Carbon Allotrope Predicted from First Principles Calculations. ChemPhysChem, 2020, 21, 59-64.	1.0	6
5	Energy barriers for collapsing large-diameter carbon nanotubes. Carbon, 2020, 159, 161-165.	5.4	9
6	Electronic properties of substitutional impurities in graphenelike <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> , <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>t</mml:mi><mml:mi>g</mml:mi><mml:mtext>â^’</mml:mtext><mml:mi mathvariant="normal">C</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant	1.1	11
7	On temperature effects on the structural phase transitions of GaP. Journal of Physics: Conference Series, 2020, 1609, 012016.	0.3	1
8	Emission redshift in DCM2-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Alq</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> caused by nonlinear Stark shifts and FÃ¶rster-mediated exciton diffusion. Physical Review B, 2020, 102, .	1.1	11
9	Pressure dependence of room-temperature structural properties of CaAl2Si2. Journal of Physics Condensed Matter, 2020, 32, 365403.	0.7	3
10	Structural and magnetic properties of a defective graphene buffer layer grown on SiC(0001): a DFT study. Physical Chemistry Chemical Physics, 2020, 22, 16096-16106.	1.3	7
11	Flat bands and gaps in twisted double bilayer graphene. Nanoscale, 2020, 12, 5014-5020.	2.8	38
12	Graphene as interface modifier in ITO and ITO-Cr electrodes. Current Applied Physics, 2020, 20, 846-852.	1.1	3
13	Exotic impurity-induced states in single-layer h -BN: The role of sublattice structure and intervalley interactions. Physical Review B, 2019, 100, .	1.1	6
14	Theoretical characterization of hexagonal 2D Be₃N₂ monolayers. New Journal of Chemistry, 2019, 43, 2933-2941.	1.4	20
15	Layer breathing and shear modes in multilayer graphene: a DFT-vdW study. Journal of Physics Condensed Matter, 2019, 31, 295301.	0.7	5
16	Novel 2D materials from exfoliation of layered hydroxide salts: A theoretical study. Applied Surface Science, 2019, 483, 762-771.	3.1	14
17	Temperature effects on the structural phase transitions of gallium phosphide. Computational Materials Science, 2019, 161, 265-275.	1.4	8
18	n-Diamondynes: Expanding the family of carbon allotropes. Carbon, 2018, 136, 337-344.	5.4	15

#	Article	IF	Citations
19	High hole-mobility of rrP3HT in organic field-effect transistors using low-polarity polyurethane gate dielectric. Organic Electronics, 2018, 58, 33-37.	1.4	15
20	Linear magnetoresistivity in layered semimetallic CaAl2Si2. Scientific Reports, 2018, 8, 4102.	1.6	4
21	Tight binding parametrization of few-layer black phosphorus from first-principles calculations. Computational Materials Science, 2018, 143, 411-417.	1.4	12
22	Photonic spin Hall effect in bilayer graphene moirÃ© superlattices. Physical Review B, 2018, 98, .	1.1	50
23	Electronic structure and optical properties of twisted multilayer graphene. Physical Review B, 2018, 98, .	1.1	23
24	Van der Waals interactions and the properties of graphite and 2H-, 3R- and 1T-MoS2: A comparative study. Computational Materials Science, 2018, 152, 146-150.	1.4	30
25	Disentangling contributions of point and line defects in the Raman spectra of graphene-related materials. 2D Materials, 2017, 4, 025039.	2.0	146
26	Investigation of organic magnetoresistance dependence on spin-orbit coupling using 8-hydroxyquinolinate rare-earth based complexes. Applied Physics Letters, 2016, 108, 203303.	1.5	1
27	Donor wave functions in Si gauged by STM images. Physical Review B, 2016, 93, .	1.1	18
28	Giant and Tunable Anisotropy of Nanoscale Friction in Graphene. Scientific Reports, 2016, 6, 31569.	1.6	41
29	Effects of edge magnetism on the Kohn anomalies of zigzag graphene nanoribbons. Nanotechnology, 2016, 27, 065707.	1.3	1
30	Boron-substitution and defects in B2-type AlNi compound: Site-preference and influence on structural, thermodynamic and electronic properties. Journal of Alloys and Compounds, 2016, 669, 210-216.	2.8	1
31	Phosphorous bonding in single wall carbon nanotubes studied by X-ray photoelectron spectroscopy and DFT calculations. Carbon, 2016, 99, 1-7.	5.4	17
32	Study of Carbon Nanostructures for Soil Fertility Improvement. Nanomedicine and Nanotoxicology, 2016, , 85-104.	0.1	1
33	Structural analysis of zeolite beta through periodic ab initio simulations of XRD and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si26.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mn>29</mml:mn></mml:mrow></mml:msup><mml:mtext>Si</mml:mtext></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si27.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mn>17</mml:mn></mml:mrow></mml:	1.8	7
34	Electronic and structural properties of vacancies and hydrogen adsorbates on trilayer graphene. Journal of Physics Condensed Matter, 2015, 27, 335302.	0.7	6
35	Systematic determination of absolute absorption cross-section of individual carbon nanotubes. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 7564-7569.	3.3	69
36	Quantifying defects in N-layer graphene via a phenomenological model of Raman spectroscopy. Nuclear Instruments & Methods in Physics Research B, 2014, 319, 71-74.	0.6	15

#	Article	IF	Citations
37	Ab initioquasiparticle band structure of ABA and ABC-stacked graphene trilayers. Physical Review B, 2014, 89, .	1.1	26
38	Chemical Analysis and Molecular Models for Calciumâ€“Oxygenâ€“Carbon Interactions in Black Carbon Found in Fertile Amazonian Anthrosoils. Environmental Science & Technology, 2014, 48, 7445-7452.	4.6	53
39	Magnetic response of zigzag nanoribbons under electric fields. Journal of Physics Condensed Matter, 2014, 26, 216002.	0.7	7
40	Resonance effects on the Raman spectra of graphene superlattices. Physical Review B, 2013, 88, .	1.1	128
41	A combined LEED and DFT surface structure determination of Cu3Au(001): Evidence of a surface stacking fault. Surface Science, 2013, 618, 167-172.	0.8	2
42	An Explicit Formula for Optical Oscillator Strength of Excitons in Semiconducting Single-Walled Carbon Nanotubes: Family Behavior. Nano Letters, 2013, 13, 54-58.	4.5	25
43	First-principles study of oxygen-induced copper segregation in Cu3Au(1 1 1). Chemical Physics, 2013, 410, 99-102.	0.9	9
44	Probing the electronic properties of ternary AnM3nâ˜1B2n (n = 1: A = Ca, Sr; M = Rh, Ir and n = 3: A = Ca,) Tj ETQq0 0 0 rgBT /Overlock 2013, 14, 035003.	2.8	2
45	Intermolecular interactions and substrate effects for an adamantane monolayer on a Au(111) surface. Physical Review B, 2013, 88, .	1.1	6
46	Molecular hyperfine fields in organic magnetoresistance devices. Physical Review B, 2013, 87, .	1.1	13
47	First-principles calculations and XPS measurements of gold segregation at the Cu3Au(111) surface. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2012, 30, 051802.	0.6	9
48	Microscopic model of a phononic refrigerator. Physical Review B, 2012, 86, .	1.1	37
49	Effects of disorder range and electronic energy on the perfect transmission in graphene nanoribbons. Physical Review B, 2012, 86, .	1.1	13
50	Half-metallicity induced by charge injection in hexagonal boron nitride clusters embedded in graphene. Physical Review B, 2012, 86, .	1.1	19
51	Production and Characterization of Boron-Doped Single Wall Carbon Nanotubes. Journal of Physical Chemistry C, 2012, 116, 3281-3285.	1.5	32
52	Ab initio studies of pristine and oxidized Cu3Au(100) and (111) surfaces. Journal of Materials Science, 2012, 47, 7594-7600.	1.7	7
53	Structural determination of stable MoOx monolayers on O/Cu3Au(100): DFT calculations. Chemical Physics, 2012, 406, 47-49.	0.9	1
54	Anomalous insulator-metal transition in boron nitride-graphene hybrid atomic layers. Physical Review B, 2012, 86, .	1.1	42

#	Article	IF	Citations
55	Structural and Phonon Properties of Bundled Single- and Double-Wall Carbon Nanotubes Under Pressure. Journal of Physical Chemistry C, 2012, 116, 22637-22645.	1.5	41
56	An atlas of carbon nanotube optical transitions. Nature Nanotechnology, 2012, 7, 325-329.	15.6	186
57	Hyperfine interactions in silicon quantum dots. Physical Review B, 2011, 83, .	1.1	87
58	Heat Pumping in Nanomechanical Systems. Physical Review Letters, 2011, 106, 135504.	2.9	20
59	Intervalley coupling for interface-bound electrons in silicon: An effective mass study. Physical Review B, 2011, 84, .	1.1	60
60	One-dimensional structural irregularities in graphene: chiral edges and grain boundaries. Journal of Physics: Conference Series, 2011, 302, 012016.	0.3	5
61	Properties of Charged Defects on Unidimensional Polymers. Journal of Computational and Theoretical Nanoscience, 2011, 8, 541-549.	0.4	5
62	Spatially resolving edge states of chiral grapheneÂnanoribbons. Nature Physics, 2011, 7, 616-620.	6.5	628
63	Theory of magnetic edge states in chiral graphene nanoribbons. Physical Review B, 2011, 84, .	1.1	113
64	Direct comparison between two structural models by DFT calculations. Journal of Solid State Chemistry, 2011, 184, 1105-1111.	1.4	66
65	Molecular Electronics Devices: A Short Review. Journal of Computational and Theoretical Nanoscience, 2010, 7, 503-516.	0.4	22
66	Quantifying ion-induced defects and Raman relaxation length in graphene. Carbon, 2010, 48, 1592-1597.	5.4	1,443
67	Measuring disorder in graphene with the G and D bands. Physica Status Solidi (B): Basic Research, 2010, 247, 2980-2982.	0.7	190
68	Gap opening by asymmetric doping in graphene bilayers. Physical Review B, 2010, 82, .	1.1	27
69	Signatures of oxygen on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>From isolated impurity to oxide regimes. Physical Review B, 2010, 82, .	1.1	2
70	Comment on â€œWave-scattering formalism for thermal conductance in thin wires with surface disorderâ€• Physical Review B, 2010, 81, .	1.1	2
71	Proposal for a single-molecule field-effect transistor for phonons. Physical Review B, 2010, 81, .	1.1	11
72	Evolution of the Raman spectra from single-, few-, and many-layer graphene with increasing disorder. Physical Review B, 2010, 82, .	1.1	606

#	Article	IF	Citations
73	Raman study of ion-induced defects inN-layer graphene. Journal of Physics Condensed Matter, 2010, 22, 334204.	0.7	110
74	Charge transfer and screening effects in polyynes encapsulated inside single-wall carbon nanotubes. Physical Review B, 2009, 80, .	1.1	33
75	Experimental and theoretical investigation of tris-(8-hydroxy-quinolinate) aluminum (Alq3) photo degradation. Organic Electronics, 2009, 10, 1417-1423.	1.4	33
76	Early stages of vanadium deposition on Si(111)-7Ã—7. Surface Science, 2009, 603, 835-838.	0.8	0
77	Electronâ^'Hole Interaction in Carbon Nanotubes: Novel Screening and Exciton Excitation Spectra. Nano Letters, 2009, 9, 1330-1334.	4.5	64
78	Quasiparticle and Excitonic Effects in the Optical Response of Nanotubes and Nanoribbons. Topics in Applied Physics, 2007, , 195-227.	0.4	22
79	Resonance Raman study of polyynes encapsulated in single-wall carbon nanotubes. Physical Review B, 2007, 76, .	1.1	51
80	Effect of post-growth annealing on the optical properties of InAs/GaAs quantum dots: A tight-binding study. Journal of Applied Physics, 2007, 102, 023711.	1.1	14
81	Chemical identification in the (100) surface using scanning tunneling microscopy and first-principles calculations. Surface Science, 2007, 601, 5540-5545.	0.8	16
82	Excitons in carbon nanotubes: Diameter and chirality trends. Physica Status Solidi (B): Basic Research, 2007, 244, 4016-4020.	0.7	35
83	Straight to the bar: Molecular nanostructures, graphene, nanotubes. XXIst International Winterschool on Electronic Properties of Novel Materials (IWEPNM 2007), Kirchberg, Austria, 10â€“17 March 2007. Physica Status Solidi - Rapid Research Letters, 2007, 1, A47-A51.	1.2	1
84	Diameter and chirality dependence of exciton properties in carbon nanotubes. Physical Review B, 2006, 74, .	1.1	179
85	Selection rules for one- and two-photon absorption by excitons in carbon nanotubes. Physical Review B, 2006, 73, .	1.1	48
86	Review on the symmetry-related properties of carbon nanotubes. Physics Reports, 2006, 431, 261-302.	10.3	138
87	Application of standard DFT theory for nonbonded interactions in soft matter: Prototype study of poly-para-phenylene. Journal of Computational Chemistry, 2006, 27, 217-227.	1.5	15
88	Temperature Dependence of the Optical Transition Energies of Carbon Nanotubes: The Role of Electron-Phonon Coupling and Thermal Expansion. Physical Review Letters, 2006, 96, 127403.	2.9	75
89	Silicon-based spin and charge quantum computation. Anais Da Academia Brasileira De Ciencias, 2005, 77, 201-222.	0.3	6
90	Family Behavior of the Pressure and Temperature Dependences of the Band Gap of Semiconducting Carbon Nanotubes. AIP Conference Proceedings, 2005, , .	0.3	0

#	Article	IF	Citations
91	Temperature Dependence of the Band Gap of Semiconducting Carbon Nanotubes. Physical Review Letters, 2005, 94, 036801.	2.9	119
92	Theory of sodium ordering inNaxCoO2. Physical Review B, 2005, 71, .	1.1	102
93	Theory andAbÂInitioCalculation of Radiative Lifetime of Excitons in Semiconducting Carbon Nanotubes. Physical Review Letters, 2005, 95, 247402.	2.9	295
94	Structural Transformations of Carbon Nanotubes under Hydrostatic Pressure. Nano Letters, 2005, 5, 2268-2273.	4.5	93
95	Hydrostatic pressure effects on the structural and electronic properties of carbon nanotubes. Physica Status Solidi (B): Basic Research, 2004, 241, 3352-3359.	0.7	88
96	Switching times in electric-field-tunable GaAs/AlAs heterostructures. Applied Physics Letters, 2002, 81, 2247-2249.	1.5	2
97	The Nature of Shallow-State Wave Functions in Semiconductors. Physica Status Solidi (B): Basic Research, 2002, 232, 106-110.	0.7	0
98	Ab initio studies of electromechanical effects in carbon nanotubes. Brazilian Journal of Physics, 2002, 32, 427-429.	0.7	1
99	Polarons in Carbon Nanotubes. Physical Review Letters, 2001, 86, 3372-3375.	2.9	67
100	An elastic model for the Inâ€“In correlations in InxGa1â^'xAs semiconductor alloys. Solid State Communications, 2000, 115, 287-290.	0.9	2
101	Tight-binding total-energy method applied to polyacetylene. Physical Review B, 2000, 61, 7187-7190.	1.1	5
102	Vacancy diffusion in silicon: analysis of transition state theory. Brazilian Journal of Physics, 1999, 29, 828-830.	0.7	1
103	Quantum well to quantum wire crossover in AlAs/GaAs/AlAs heterostructures induced by interface roughness increase. Brazilian Journal of Physics, 1999, 29, 834-838.	0.7	1
104	Segregation, interface morphology, and the optical properties ofGaAs/AlAsquantum wells: A theoretical study. Physical Review B, 1999, 60, 1787-1791.	1.1	14
105	Semiconductor Hetrostructures with Non-Ideal Interfaces: Electronic Structure and Optical Properties. Physica Status Solidi A, 1999, 173, 235-246.	1.7	2
106	Tight-binding scheme for impurity states in semiconductors. Physical Review B, 1999, 59, 2722-2725.	1.1	18
107	Role of Interface Imperfections on Intervalley Coupling in GaAs/AlAs Superlattices. Physical Review Letters, 1999, 83, 2034-2037.	2.9	14
108	Disorder and size effects in the envelope-function approximation. Physical Review B, 1997, 56, 9625-9629.	1.1	35

#	Article	IF	Citations
109	Direct-to-Indirect Crossover in Semiconductor Alloys: A First-Order Phase Transition?. Physical Review Letters, 1995, 74, 769-772.	2.9	22
110	Partial-ordering effects inInxGa1â^'xP. Physical Review B, 1993, 47, 4044-4047.	1.1	24
111	Pressure and composition effects on the gap properties of AlxGa1â^'xAs. Journal of Applied Physics, 1993, 74, 5531-5537.	1.1	26
112	Physical criteria for the directâ€toâ€indirect gap crossover in AlxGa1â^'xAs alloys. Applied Physics Letters, 1992, 60, 704-706.	1.5	7
113	Gap states and localization properties of one-dimensional Fibonacci quasicrystals. Physical Review B, 1990, 42, 6402-6407.	1.1	48
114	Growth-driven ordering and anisotropy in semiconductor alloys. Physical Review B, 1989, 40, 8299-8304.	1.1	6