

Claudio Attaccalite

List of Publications by Year in descending order

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Version: 2024-02-01

60
papers

4,198
citations

147566

31
h-index

128067

60
g-index

66
all docs

66
docs citations

66
times ranked

4399
citing authors

#	ARTICLE	IF	CITATIONS
1	Correlation Energy and Spin Polarization in the 2D Electron Gas. Physical Review Letters, 2002, 88, 256601.	2.9	366
2	First-principles GW calculations for fullerenes, porphyrins, phtalocyanine, and other molecules of interest for organic photovoltaic applications. Physical Review B, 2011, 83, .	1.1	362
3	Many-body perturbation theory calculations using the yambo code. Journal of Physics Condensed Matter, 2019, 31, 325902.	0.7	269
4	Impact of the electron-electron correlation on phonon dispersion: Failure of LDA and GGA DFT functionals in graphene and graphite. Physical Review B, 2008, 78, .	1.1	257
5	Tight-binding description of the quasiparticle dispersion of graphite and few-layer graphene. Physical Review B, 2008, 78, .	1.1	243
6	Correlated geminal wave function for molecules: An efficient resonating valence bond approach. Journal of Chemical Physics, 2004, 121, 7110-7126.	1.2	189
7	Strong Charge-Transfer Excitonic Effects and the Bose-Einstein Exciton Condensate in Graphane. Physical Review Letters, 2010, 104, 226804.	2.9	180
8	Coupling of excitons and defect states in boron-nitride nanostructures. Physical Review B, 2011, 83, .	1.1	177
9	First-principles GW calculations for DNA and RNA nucleobases. Physical Review B, 2011, 83, .	1.1	152
10	Charge-transfer excitations in molecular donor-acceptor complexes within the many-body Bethe-Salpeter approach. Applied Physics Letters, 2011, 99, .	1.5	142
11	Stable Liquid Hydrogen at High Pressure by a Novel <i>Ab Initio</i> Molecular-Dynamics Calculation. Physical Review Letters, 2008, 100, 114501.	2.9	113
12	Electron-Electron Correlation in Graphite: A Combined Angle-Resolved Photoemission and First-Principles Study. Physical Review Letters, 2008, 100, 037601.	2.9	103
13	Real-time approach to the optical properties of solids and nanostructures: Time-dependent Bethe-Salpeter equation. Physical Review B, 2011, 84, .	1.1	103
14	Excited states properties of organic molecules: from density functional theory to the GW and Bethe-Salpeter Green's function formalisms. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130271.	1.6	100
15	Second harmonic generation in h-BN and MoS ₂ monolayers: Role of electron-hole interaction. Physical Review B, 2014, 89, .	1.1	97
16	Doped Graphene as Tunable Electron-Phonon Coupling Material. Nano Letters, 2010, 10, 1172-1176.	4.5	84
17	Phonon surface mapping of graphite: Disentangling quasi-degenerate phonon dispersions. Physical Review B, 2009, 80, .	1.1	83
18	Electronic structure and electron-phonon coupling of doped graphene layers in KC_8 . Physical Review B, 2009, 79, .	1.1	81

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19	Strong electronic correlation in the hydrogen chain: A variational Monte Carlo study. Physical Review B, 2011, 84, .	1.1	73
20	Angle-resolved photoemission study of the graphite intercalation compound KC8: A key to graphene. Physical Review B, 2009, 80, .	1.1	69
21	Comment on "Huge Excitonic Effects in Layered Hexagonal Boron Nitride". Physical Review Letters, 2008, 100, 189701; discussion 189702.	2.9	64
22	Direct and indirect excitons in boron nitride polymorphs: A story of atomic configuration and electronic correlation. Physical Review B, 2018, 98, .	1.1	63
23	Nonlinear optics from an <i>ab initio</i> approach by means of the dynamical Berry phase: Application to second- and third-harmonic generation in semiconductors. Physical Review B, 2013, 88, .	1.1	62
24	Many-body Green's function <i>GW</i> and Bethe-Salpeter study of the optical excitations in a paradigmatic model dipeptide. Journal of Chemical Physics, 2013, 139, 194308.	1.2	52
25	Fermi velocity renormalization in doped graphene. Physica Status Solidi (B): Basic Research, 2009, 246, 2523-2526.	0.7	47
26	Strong second harmonic generation in SiC, ZnO, GaN two-dimensional hexagonal crystals from first-principles many-body calculations. Physical Chemistry Chemical Physics, 2015, 17, 9533-9540.	1.3	47
27	Theory of phonon-assisted luminescence in solids: Application to hexagonal boron nitride. Physical Review B, 2019, 99, .	1.1	46
28	Speeding up the solution of the Bethe-Salpeter equation by a double-grid method and Wannier interpolation. Physical Review B, 2012, 86, .	1.1	42
29	<i>TurboRVB</i> : A many-body toolkit for <i>ab initio</i> electronic simulations by quantum Monte Carlo. Journal of Chemical Physics, 2020, 152, 204121.	1.2	37
30	Exploring approximations to the <i>GW</i> self-energy ionic gradients. Physical Review B, 2015, 91, .	1.1	32
31	Electron-phonon coupling and charge-transfer excitations in organic systems from many-body perturbation theory. Journal of Materials Science, 2012, 47, 7472-7481.	1.7	31
32	Excitonic effects in third-harmonic generation: The case of carbon nanotubes and nanoribbons. Physical Review B, 2017, 95, .	1.1	27
33	Optical properties of Cu-chalcogenide photovoltaic absorbers from self-consistent GW the Bethe-Salpeter equation. Physical Review B, 2015, 91, .	1.1	24
34	Exciton interference in hexagonal boron nitride. Physical Review B, 2018, 97, .	1.1	23
35	Second-harmonic generation in single-layer monochalcogenides: A response from first-principles real-time simulations. Physical Review Materials, 2019, 3, .	0.9	23
36	Absorption of BN nanotubes under the influence of a perpendicular electric field. Physica Status Solidi (B): Basic Research, 2007, 244, 4288-4292.	0.7	22

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37	Efficient Gate-tunable light-emitting device made of defective boron nitride nanotubes: from ultraviolet to the visible. <i>Scientific Reports</i> , 2013, 3, 2698.	1.6	22
38	Optical properties of periodic systems within the current-current response framework: Pitfalls and remedies. <i>Physical Review B</i> , 2017, 95, .	1.1	22
39	Two-photon absorption in two-dimensional materials: The case of hexagonal boron nitride. <i>Physical Review B</i> , 2018, 98, .	1.1	22
40	Properties of Gutzwiller wave functions for multiband models. <i>Physical Review B</i> , 2003, 68, .	1.1	21
41	Dielectrics in a time-dependent electric field: A real-time approach based on density-polarization functional theory. <i>Physical Review B</i> , 2016, 94, .	1.1	20
42	Angle-resolved electron energy loss spectroscopy in hexagonal boron nitride. <i>Physical Review B</i> , 2017, 96, .	1.1	18
43	Resonating-valence-bond ground state of lithium nanoclusters. <i>Physical Review B</i> , 2009, 79, .	1.1	16
44	Structural, electronic, and optical properties of the C-C complex in bulk silicon from first principles. <i>Journal of Applied Physics</i> , 2018, 123, .	1.1	16
45	Strongly Bound Excitons in Metal-Organic Framework MOF-5: A Many-Body Perturbation Theory Study. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4045-4051.	2.1	15
46	Ellipsometry Study of Hexagonal Boron Nitride Using Synchrotron Radiation: Transparency Window in the Far-UV. <i>Advanced Photonics Research</i> , 2021, 2, 2000101.	1.7	14
47	Two-dimensional electron gas: Correlation energy versus density and spin polarization. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 126-130.	1.0	13
48	Performance of polarisation functionals for linear and nonlinear optical properties of bulk zinc chalcogenides ZnX (X = S, Se, and Te). <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21179-21189.	1.3	13
49	Influence of halogen substitution on aggregation-induced near infrared emission of boron difluoride complexes of 2-hydroxychalcones. <i>Materials Chemistry Frontiers</i> , 2019, 3, 86-92.	3.2	9
50	Bethe-Salpeter Study of the Optical Absorption of <i>trans</i> and <i>cis</i> Azobenzene-Functionalized Metal-Organic Frameworks Using Molecular and Periodic Models. <i>Journal of Physical Chemistry C</i> , 2021, 125, 7401-7412.	1.5	9
51	Preparation and electronic properties of potassium doped graphite single crystals. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 2072-2076.	0.7	8
52	Tuning the Direct and Indirect Excitonic Transitions of <i>h</i> -BN by Hydrostatic Pressure. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12880-12885.	1.5	8
53	Comment on "Electronic Structure of Superconducting KC8 and Nonsuperconducting LiC6 Graphite Intercalation Compounds: Evidence for a Graphene-Sheet-Driven Superconducting State": <i>Physical Review Letters</i> , 2012, 108, 149701; discussion 149702.	2.9	7
54	Resonating valence bond wave function: from lattice models to realistic systems. <i>Computer Physics Communications</i> , 2005, 169, 386-393.	3.0	6

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55	Low energy quasiparticle dispersion of graphite by angle-resolved photoemission spectroscopy. Physica Status Solidi (B): Basic Research, 2007, 244, 4129-4133.	0.7	5
56	Nonlinear optical response of ferroelectric oxides: First-principles calculations within the time and frequency domains. Physical Review Materials, 2022, 6, .	0.9	5
57	Tetraphenyl Tetrel Molecules and Molecular Crystals: From Structural Properties to Nonlinear Optics. Journal of Physical Chemistry C, 2022, 126, 3713-3726.	1.5	4
58	Excitons under strain: light absorption and emission in strained hexagonal boron nitride. SciPost Physics, 2022, 12, .	1.5	4
59	Ab Initio Study of Graphene/hBN Van der Waals Heterostructures: Effect of Electric Field, Twist Angles and p-n Doping on the Electronic Properties. Nanomaterials, 2022, 12, 2118.	1.9	1
60	Response to "Comment on "Structural, electronic, and optical properties of the C-C complex in bulk silicon from first principles" [J. Appl. Phys. 124, 086101 (2018)]. Journal of Applied Physics, 2018, 124, 086102.	1.1	0