Claudio Attaccalite

List of Publications by Year
in descending order

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Version: 2024-02-01

60	4,198	147726	128225
papers	citations	31 h-index	60 g-index

66	66	66	4399
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Tetraphenyl Tetrel Molecules and Molecular Crystals: From Structural Properties to Nonlinear Optics. Journal of Physical Chemistry C, 2022, 126, 3713-3726.	1.5	4
2	Excitons under strain: light absorption and emission in strained hexagonal boron nitride. SciPost Physics, 2022, 12, .	1.5	4
3	Nonlinear optical response of ferroelectric oxides: First-principles calculations within the time and frequency domains. Physical Review Materials, 2022, 6, .	0.9	5
4	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
5	Ellipsometry Study of Hexagonal Boron Nitride Using Synchrotron Radiation: Transparency Window in the Farâ€UVC. Advanced Photonics Research, 2021, 2, 2000101.	1.7	14
6	Betheâ€“Salpeter Study of the Optical Absorption of trans and cis Azobenzene-Functionalized Metalâ€“Organic Frameworks Using Molecular and Periodic Models. Journal of Physical Chemistry C, 2021, 125, 7401-7412.	1.5	9
7	Strongly Bound Excitons in Metalâ€“Organic Framework MOF-5: A Many-Body Perturbation Theory Study. Journal of Physical Chemistry Letters, 2021, 12, 4045-4051.	2.1	15
8	Tuning the Direct and Indirect Excitonic Transitions of h-BN by Hydrostatic Pressure. Journal of Physical Chemistry C, 2021, 125, 12880-12885.	1.5	8
9	<scp>TurboRVB</scp>: A many-body toolkit for ab initio electronic simulations by quantum Monte Carlo. Journal of Chemical Physics, 2020, 152, 204121.	1.2	37
10	Influence of halogen substitution on aggregation-induced near infrared emission of borondifluoride complexes of 2â€²-hydroxychalcones. Materials Chemistry Frontiers, 2019, 3, 86-92.	3.2	9
11	Many-body perturbation theory calculations using the yambo code. Journal of Physics Condensed Matter, 2019, 31, 325902.	0.7	269
12	Theory of phonon-assisted luminescence in solids: Application to hexagonal boron nitride. Physical Review B, 2019, 99, .	1.1	46
13	Second-harmonic generation in single-layer monochalcogenides: A response from first-principles real-time simulations. Physical Review Materials, 2019, 3, .	0.9	23
14	Exciton interference in hexagonal boron nitride. Physical Review B, 2018, 97, .	1.1	23
15	Structural, electronic, and optical properties of the C-C complex in bulk silicon from first principles. Journal of Applied Physics, 2018, 123, .	1.1	16
16	Direct and indirect excitons in boron nitride polymorphs: A story of atomic configuration and electronic correlation. Physical Review B, 2018, 98, .	1.1	63
17	Two-photon absorption in two-dimensional materials: The case of hexagonal boron nitride. Physical Review B, 2018, 98, .	1.1	22
18	Response to â€œComment on â€˜Structural, electronic, and optical properties of the C-C complex in bulk silicon from first principlesâ€™â€•[J. Appl. Phys. 124, 086101 (2018)]. Journal of Applied Physics, 2018, 124, 086102.	1.1	0

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19	Excitonic effects in third-harmonic generation: The case of carbon nanotubes and nanoribbons. Physical Review B, 2017, 95, .	1.1	27
20	Angle-resolved electron energy loss spectroscopy in hexagonal boron nitride. Physical Review B, 2017, 96, .	1.1	18
21	Optical properties of periodic systems within the current-current response framework: Pitfalls and remedies. Physical Review B, 2017, 95, .	1.1	22
22	Performance of polarisation functionals for linear and nonlinear optical properties of bulk zinc chalcogenides ZnX (X = S, Se, and Te). Physical Chemistry Chemical Physics, 2016, 18, 21179-21189.	1.3	13
23	Dielectrics in a time-dependent electric field: A real-time approach based on density-polarization functional theory. Physical Review B, 2016, 94, .	1.1	20
24	Exploring approximations to theGWself-energy ionic gradients. Physical Review B, 2015, 91, .	1.1	32
25	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
26	Optical properties of Cu-chalcogenide photovoltaic absorbers from self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:n the Bethe-Salpeter equation. Physical Review B, 2015, 91, .	1.1	24
27	Excited states properties of organic molecules: from density functional theory to the GW and Betheâ€“Salpeter Green's function formalisms. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130271.	1.6	100
28	Second harmonic generation in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>h</mml:mi></mml:math>-BN and MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>monolayers: Role of electron-hole interaction. Physical Review B, 2014, 89, .	1.1	97
29	Many-body Green's function GW and Bethe-Salpeter study of the optical excitations in a paradigmatic model dipeptide. Journal of Chemical Physics, 2013, 139, 194308.	1.2	52
30	Efficient Gate-tunable light-emitting device made of defective boron nitride nanotubes: from ultraviolet to the visible. Scientific Reports, 2013, 3, 2698.	1.6	22
31	Nonlinear optics from anab initioapproach by means of the dynamical Berry phase: Application to second- and third-harmonic generation in semiconductors. Physical Review B, 2013, 88, .	1.1	62
32	Comment on â€œElectronic Structure of SuperconductingKC8and NonsuperconductingLiC6Graphite Intercalation Compounds: Evidence for a Graphene-Sheet-Driven Superconducting Stateâ€• Physical Review Letters, 2012, 108, 149701; discussion 149702.	2.9	7
33	Electronâ€“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
34	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
35	First-principles<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="italic">GW</mml:mi></mml:mrow></mml:math>calculations for fullerenes, porphyrins, phtalocyanine, and other molecules of interest for organic photovoltaic applications. Physical Review B, 2011, 83, .	1.1	362
36	Coupling of excitons and defect states in boron-nitride nanostructures. Physical Review B, 2011, 83, .	1.1	177

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37	First-principlesGWcalculations for DNA and RNA nucleobases. Physical Review B, 2011, 83, .	1.1	152
38	Charge-transfer excitations in molecular donor-acceptor complexes within the many-body Bethe-Salpeter approach. Applied Physics Letters, 2011, 99, .	1.5	142
39	Real-time approach to the optical properties of solids and nanostructures: Time-dependent Bethe-Salpeter equation. Physical Review B, 2011, 84, .	1.1	103
40	Strong electronic correlation in the hydrogen chain: A variational Monte Carlo study. Physical Review B, 2011, 84, .	1.1	73
41	Doped Graphene as Tunable Electronâ^'Phonon Coupling Material. Nano Letters, 2010, 10, 1172-1176.	4.5	84
42	Strong Charge-Transfer Excitonic Effects and the Bose-Einstein Exciton Condensate in Graphane. Physical Review Letters, 2010, 104, 226804.	2.9	180
43	Resonating-valence-bond ground state of lithium nanoclusters. Physical Review B, 2009, 79, .	1.1	16
44	Electronic structure and electron-phonon coupling of doped graphene layers in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>KC</mml:mtext></mml:mrow><mml:mn>8</mml:mn></mml:msu Physical Review B, 2009, 79, .	1.1	81
45	Fermi velocity renormalization in doped graphene. Physica Status Solidi (B): Basic Research, 2009, 246, 2523-2526.	0.7	47
46	Phonon surface mapping of graphite: Disentangling quasi-degenerate phonon dispersions. Physical Review B, 2009, 80, .	1.1	83
47	Angle-resolved photoemission study of the graphite intercalation compoundKC8: A key to graphene. Physical Review B, 2009, 80, .	1.1	69
48	Preparation and electronic properties of potassium doped graphite single crystals. Physica Status Solidi (B): Basic Research, 2008, 245, 2072-2076.	0.7	8
49	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
50	Stable Liquid Hydrogen at High Pressure by a NovelAbÂInitioMolecular-Dynamics Calculation. Physical Review Letters, 2008, 100, 114501.	2.9	113
51	Tight-binding description of the quasiparticle dispersion of graphite and few-layer graphene. Physical Review B, 2008, 78, .	1.1	243
52	Electron-Electron Correlation in Graphite: A Combined Angle-Resolved Photoemission and First-Principles Study. Physical Review Letters, 2008, 100, 037601.	2.9	103
53	Comment on â€œHuge Excitonic Effects in Layered Hexagonal Boron Nitrideâ€• Physical Review Letters, 2008, 100, 189701; discussion 189702.	2.9	64
54	Low energy quasiparticle dispersion of graphite by angleâ€•resolved photoemission spectroscopy. Physica Status Solidi (B): Basic Research, 2007, 244, 4129-4133.	0.7	5

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55	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
56	Resonating valence bond wave function: from lattice models to realistic systems. Computer Physics Communications, 2005, 169, 386-393.	3.0	6
57	Correlated geminal wave function for molecules:â€,An efficient resonating valence bond approach. Journal of Chemical Physics, 2004, 121, 7110-7126.	1.2	189
58	Two-dimensional electron gas: Correlation energy versus density and spin polarization. International Journal of Quantum Chemistry, 2003, 91, 126-130.	1.0	13
59	Properties of Gutzwiller wave functions for multiband models. Physical Review B, 2003, 68, .	1.1	21
60	Correlation Energy and Spin Polarization in the 2D Electron Gas. Physical Review Letters, 2002, 88, 256601.	2.9	366