Xavier Blase

List of Publications by Year
in descending order

111 papers	14,531 citations	28272 55 h-index	26610 107 g-index
112 all docs	112 docs citations	112 times ranked	12245 citing authors

#	Article	IF	Citations
1	Stability and Band Gap Constancy of Boron Nitride Nanotubes. Europhysics Letters, 1994, 28, 335-340.	2.0	1,406
2	Electronic and transport properties of nanotubes. Reviews of Modern Physics, 2007, 79, 677-732.	45.6	1,234
3	Giant osmotic energy conversion measured in a single transmembrane boron nitride nanotube. Nature, 2013, 494, 455-458.	27.8	937
4	Hybridization effects and metallicity in small radius carbon nanotubes. Physical Review Letters, 1994, 72, 1878-1881.	7.8	931
5	Identification of Electron Donor States in N-Doped Carbon Nanotubes. Nano Letters, 2001, 1, 457-460.	9.1	727
6	Quasiparticle band structure of bulk hexagonal boron nitride and related systems. Physical Review B, 1995, 51, 6868-6875.	3.2	583
7	Synthesis ofBxCyNznanotubules. Physical Review B, 1995, 51, 11229-11232.	3.2	413
8	N-doping and coalescence of carbon nanotubes: synthesis and electronic properties. Applied Physics A: Materials Science and Processing, 2002, 74, 355-361.	2.3	392
9	Quasiparticle band structures of six II-VI compounds: ZnS, ZnSe, ZnTe, CdS, CdSe, and CdTe. Physical Review B, 1994, 50, 10780-10787.	3.2	366
10	Electronic Structure and Localized States at Carbon Nanotube Tips. Physical Review Letters, 1997, 78, 2811-2814.	7.8	355
11	Effects of Nanodomain Formation on the Electronic Structure of Doped Carbon Nanotubes. Physical Review Letters, 1998, 81, 2332-2335.	7.8	305
12	Theory of composite BxCyNz nanotube heterojunctions. Applied Physics Letters, 1997, 70, 197-199.	3.3	243
13	Superconductivity in doped cubic silicon. Nature, 2006, 444, 465-468.	27.8	238
14	Microscopic Growth Mechanisms for Carbon Nanotubes. Science, 1997, 275, 647-649.	12.6	220
15	0â€“0 Energies Using Hybrid Schemes: Benchmarks of TD-DFT, CIS(D), ADC(2), CC2, and BSE/GW formalisms for 80 Real-Life Compounds. Journal of Chemical Theory and Computation, 2015, 11, 5340-5359.	5.3	208
16	Ab InitioPhotoabsorption Spectra and Structures of Small Semiconductor and Metal Clusters. Physical Review Letters, 1996, 77, 247-250.	7.8	193
17	Benchmarking the Betheâ€“Salpeter Formalism on a Standard Organic Molecular Set. Journal of Chemical Theory and Computation, 2015, 11, 3290-3304.	5.3	172
18	Surface Segregation and Backscattering in Doped Silicon Nanowires. Physical Review Letters, 2006, 96, 166805.	7.8	166

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19	Role of the Dopant in the Superconductivity of Diamond. Physical Review Letters, 2004, 93, 237004.	7.8	164
20	Ionic Cohesion and Electron Doping of Thin Carbon Tubules with Alkali Atoms. Physical Review Letters, 1995, 74, 2993-2996.	7.8	163
21	Synthesis and Structure of Silicon-doped Heterofullerenes. Physical Review Letters, 1998, 80, 5365-5368.	7.8	163
22	Frustration Effects and Microscopic Growth Mechanisms for BN Nanotubes. Physical Review Letters, 1998, 80, 1666-1669.	7.8	163
23	Superconducting group-IV semiconductors. Nature Materials, 2009, 8, 375-382.	27.5	161
24	The Betheâ€“Salpeter equation in chemistry: relations with TD-DFT, applications and challenges. Chemical Society Reviews, 2018, 47, 1022-1043.	38.1	158
25	Electronic structure and its dependence on local order for H/Si(111)-(1Ã—1) surfaces. Physical Review Letters, 1993, 70, 1992-1995.	7.8	153
26	High Pressure Behavior of Silicon Clathrates: A New Class of Low Compressibility Materials. Physical Review Letters, 1999, 83, 5290-5293.	7.8	146
27	Boron-nitride and boron-carbonitride nanotubes: synthesis, characterization and theory. Advances in Physics, 2010, 59, 101-179.	14.4	143
28	Charge-transfer excitations in molecular donor-acceptor complexes within the many-body Bethe-Salpeter approach. Applied Physics Letters, 2011, 99, .	3.3	142
29	Superconductivity in Dopedsp3Semiconductors: The Case of the Clathrates. Physical Review Letters, 2003, 91, 247001.	7.8	136
30	Structural and electronic properties of composite B x C y N z nanotubes and heterojunctions. Applied Physics A: Materials Science and Processing, 1999, 68, 293-300.	2.3	132
31	Chemically Induced Mobility Gaps in Graphene Nanoribbons: A Route for Upscaling Device Performances. Nano Letters, 2009, 9, 2725-2729.	9.1	120
32	Boron-Mediated Growth of Long Helicity-Selected Carbon Nanotubes. Physical Review Letters, 1999, 83, 5078-5081.	7.8	119
33	Effect of the Chemical Functionalization on Charge Transport in Carbon Nanotubes at the Mesoscopic Scale. Nano Letters, 2009, 9, 940-944.	9.1	118
34	Exceptional Ideal Strength of Carbon Clathrates. Physical Review Letters, 2004, 92, 215505.	7.8	107
35	Photolysis experiments on SiC mixed clusters: From silicon carbide clusters to silicon-doped fullerenes. Journal of Chemical Physics, 1999, 110, 6927-6938.	3.0	102
36	Conductance, Surface Traps, and Passivation in Doped Silicon Nanowires. Nano Letters, 2006, 6, 2674-2678.	9.1	100

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37	Benchmark Many-Body GW and Betheâ€“Salpeter Calculations for Small Transition Metal Molecules. Journal of Chemical Theory and Computation, 2014, 10, 3934-3943.	5.3	98
38	Short-Range to Long-Range Charge-Transfer Excitations in the Zincbacteriochlorin-Bacteriochlorin Complex: A Bethe-Salpeter Study. Physical Review Letters, 2012, 109, 167801.	7.8	97
39	The Betheâ€“Salpeter Equation Formalism: From Physics to Chemistry. Journal of Physical Chemistry Letters, 2020, 11, 7371-7382.	4.6	96
40	Theoretical study of one-dimensional chains of metal atoms in nanotubes. Physical Review B, 1996, 53, 4023-4026.	3.2	93
41	Thermal Stability of Graphene and Nanotube Covalent Functionalization. Nano Letters, 2008, 8, 3315-3319.	9.1	91
42	Self-energy effects on the surface-state energies of H-Si(111)1Ã—1. Physical Review B, 1994, 49, 4973-4980.	3.2	89
43	Fast and Accurate Electronic Excitations in Cyanines with the Many-Body Betheâ€“Salpeter Approach. Journal of Chemical Theory and Computation, 2014, 10, 1212-1218.	5.3	88
44	An analytical model for the thermal conductivity of silicon nanostructures. Journal of Applied Physics, 2005, 97, 104318.	2.5	82
45	Is the Betheâ€“Salpeter Formalism Accurate for Excitation Energies? Comparisons with TD-DFT, CASPT2, and EOM-CCSD. Journal of Physical Chemistry Letters, 2017, 8, 1524-1529.	4.6	78
46	Structure and Energy of the90Â°Partial Dislocation in Diamond: A CombinedAb Initioand Elasticity Theory Analysis. Physical Review Letters, 2000, 84, 5780-5783.	7.8	75
47	Combining the Many-Body GW Formalism with Classical Polarizable Models: Insights on the Electronic Structure of Molecular Solids. Journal of Physical Chemistry Letters, 2016, 7, 2814-2820.	4.6	70
48	LOW-DIMENSIONAL QUANTUM TRANSPORT PROPERTIES OF CHEMICALLY-DISORDERED CARBON NANOTUBES: FROM WEAK TO STRONG LOCALIZATION REGIMES. Modern Physics Letters B, 2007, 21, 1955-1982.	1.9	65
49	Benchmark of Bethe-Salpeter for Triplet Excited-States. Journal of Chemical Theory and Computation, 2017, 13, 767-783.	5.3	65
50	Tailoring Band Gap and Hardness by Intercalation: Anab initioStudy ofI8@Siâ˜†46and Related Doped Clathrates. Physical Review Letters, 2001, 87, 206405.	7.8	64
51	Host dependence of the electron affinity of molecular dopants. Materials Horizons, 2019, 6, 107-114.	12.2	64
52	First principles study of gold adsorption and diffusion on graphite. Surface Science, 2004, 564, 173-178.	1.9	63
53	Anharmonicity and Lifetime of the CH Stretch Mode on Diamond H/C(111)-(1 Ã— 1). Europhysics Letters, 1995, 30, 399-404.	2.0	62
54	Orientation dependent molecular electrostatics drives efficient charge generation in homojunction organic solar cells. Nature Communications, 2020, 11, 4617.	12.8	60

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55	First Principles Calculations of Charge Transfer Excitations in Polymerâ€“Fullerene Complexes: Influence of Excess Energy. Advanced Functional Materials, 2015, 25, 1972-1984.	14.9	59
56	Molecular Fingerprints in the Electronic Properties of Crystalline Organic Semiconductors: From Experiment to Theory. Physical Review Letters, 2012, 108, 256401.	7.8	57
57	The Betheâ€“Salpeter formalism with polarisable continuum embedding: reconciling linear-response and state-specific features. Chemical Science, 2018, 9, 4430-4443.	7.4	55
58	Many-body Green's function study of coumarins for dye-sensitized solar cells. Physical Review B, 2012, 86, .	3.2	51
59	Reference Energies for Intramolecular Charge-Transfer Excitations. Journal of Chemical Theory and Computation, 2021, 17, 3666-3686.	5.3	51
60	Cubic-Scaling All-Electron GW Calculations with a Separable Density-Fitting Spaceâ€“Time Approach. Journal of Chemical Theory and Computation, 2021, 17, 2383-2393.	5.3	50
61	Quantum transport properties of chemically functionalized long semiconducting carbon nanotubes. Nano Research, 2010, 3, 288-295.	10.4	48
62	Robust Analytic-Continuation Approach to Many-Body GW Calculations. Journal of Chemical Theory and Computation, 2020, 16, 1742-1756.	5.3	47
63	Properties of composite BxCyNz nanotubes and related heterojunctions. Computational Materials Science, 2000, 17, 107-114.	3.0	46
64	Resonant hot charge-transfer excitations in fullerene-porphyrin complexes: Many-body Bethe-Salpeter study. Physical Review B, 2013, 87, .	3.2	46
65	Combining the GW formalism with the polarizable continuum model: A state-specific non-equilibrium approach. Journal of Chemical Physics, 2016, 144, 164106.	3.0	46
66	Accurate description of charged excitations in molecular solids from embedded many-body perturbation theory. Physical Review B, 2018, 97, .	3.2	46
67	Assessment of the Accuracy of the Betheâ€“Salpeter (BSE/GW) Oscillator Strengths. Journal of Chemical Theory and Computation, 2016, 12, 3969-3981.	5.3	44
68	Separable resolution-of-the-identity with all-electron Gaussian bases: Application to cubic-scaling RPA. Journal of Chemical Physics, 2019, 150, 174120.	3.0	43
69	Correlated electron-hole mechanism for molecular doping in organic semiconductors. Physical Review Materials, 2017, 1, .	2.4	42
70	Quasiparticle Effects on Tunneling Currents: A Study ofC2H4Adsorbed on theSi(001)-(2Ã—1)Surface. Physical Review Letters, 2001, 86, 2110-2113.	7.8	41
71	GW and Bethe-Salpeter study of small water clusters. Journal of Chemical Physics, 2016, 144, 034109.	3.0	38
72	Mixed-space formalism for the dielectric response in periodic systems. Physical Review B, 1995, 52, R2225-R2228.	3.2	37

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73	Guest displacement in silicon clathrates. Physical Review B, 2004, 69, .	3.2	36
74	Superconductivity in doped cubic silicon: An ab initio study. Applied Physics Letters, 2007, 90, 142511.	3.3	36
75	Electronic signature of the pentagonal rings in silicon clathrate phases: Comparison with cluster-assembled films. Physical Review B, 1998, 58, 12590-12593.	3.2	35
76	GWstudy of the metal-insulator transition of bcc hydrogen. Physical Review B, 2002, 66, .	3.2	35
77	High pressure synthesis and properties of intercalated silicon clathrates. Journal of Physics and Chemistry of Solids, 2006, 67, 1117-1121.	4.0	35
78	Combining the Betheâ€“Salpeter Formalism with Time-Dependent DFT Excited-State Forces to Describe Optical Signatures: NBO Fluoroborates as Working Examples. Journal of Chemical Theory and Computation, 2014, 10, 4548-4556.	5.3	34
79	Electronâ€“phonon coupling and charge-transfer excitations in organic systems from many-body perturbation theory. Journal of Materials Science, 2012, 47, 7472-7481.	3.7	31
80	Does Excess Energy Assist Photogeneration in an Organic Lowâ€Bandgap Solar Cell?. Advanced Functional Materials, 2015, 25, 1287-1295.	14.9	31
81	Ab Initio Calculations of Open-Cell Voltage in Li-Ion Organic Radical Batteries. Journal of Physical Chemistry C, 2015, 119, 23373-23378.	3.1	31
82	Ab initio many-body <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:m correlations in the electronic structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaNiO</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2020, 101, .	3.2	31
83	Carbon nanotube chemistry and assembly for electronic devices. Comptes Rendus Physique, 2009, 10, 330-347.	0.9	28
84	Theoretical Models for the Optical Properties of Clusters and Nanostructures. International Journal of Modern Physics B, 1997, 11, 2727-2776.	2.0	25
85	Hybrid and Constrained Resolution-of-Identity Techniques for Coulomb Integrals. Journal of Chemical Theory and Computation, 2017, 13, 1199-1208.	5.3	25
86	Pros and Cons of the Betheâ€“Salpeter Formalism for Ground-State Energies. Journal of Physical Chemistry Letters, 2020, 11, 3536-3545.	4.6	23
87	Helium Atom Excitations by the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:math> and Bethe-Salpeter Many-Body Formalism. Physical Review Letters, 2017, 118, 163001.	7.8	22
88	Bethe-Salpeter study of cationic dyes: Comparisons with ADC(2) and TD-DFT. Journal of Chemical Physics, 2017, 146, 034301.	3.0	21
89	Calculations of nâ†'Ï€* Transition Energies: Comparisons Between TD-DFT, ADC, CC, CASPT2, and BSE/GW Descriptions. Journal of Physical Chemistry A, 2017, 121, 6122-6134.	2.5	21
90	Dynamical correction to the Betheâ€“Salpeter equation beyond the plasmon-pole approximation. Journal of Chemical Physics, 2020, 153, 114120.	3.0	21

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91	Assessment of the convergence of partially self-consistent BSE/GW calculations. Molecular Physics, 2016, 114, 957-967.	1.7	19
92	Modeling the Photochromeâ€“TiO₂ Interface with Betheâ€“Salpeter and Time-Dependent Density Functional Theory Methods. Journal of Physical Chemistry Letters, 2017, 8, 936-940.	4.6	19
93	Tuning Optical Properties of Dibenzochrysenes by Functionalization: A Many-Body Perturbation Theory Study. Journal of Physical Chemistry C, 2017, 121, 24480-24488.	3.1	18
94	Photoluminescent properties of the carbon-dimer defect in hexagonal boron-nitride: A many-body finite-size cluster approach. Physical Review Materials, 2021, 5, .	2.4	16
95	Strongly Bound Excitons in Metalâ€“Organic Framework MOF-5: A Many-Body Perturbation Theory Study. Journal of Physical Chemistry Letters, 2021, 12, 4045-4051.	4.6	15
96	Quasiparticle band structure of lanthanum hydride. Physical Review B, 2001, 64, .	3.2	14
97	Ground-state correlation energy of beryllium dimer by the Bethe-Salpeter equation. SciPost Physics, 2020, 8, .	4.9	12
98	Accurate Prediction of the S₁ Excitation Energy in Solvated Azobenzene Derivatives via Embedded Orbital-Tuned Bethe-Salpeter Calculations. Journal of Chemical Theory and Computation, 2020, 16, 2021-2027.	5.3	10
99	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.	3.1	9
100	Dopingâ€Induced Dielectric Catastrophe Prompts Freeâ€Carrier Release in Organic Semiconductors. Advanced Materials, 2022, 34, e2105376.	21.0	9
101	Universal polarization energies for defects in monolayer, surface, and bulk hexagonal boron nitride: A finite-size fragments <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></mm approach. Physical Review Materials, 2022, 6, .	2.4	9
102	Doping of semicrystalline conjugated polymers: dopants within alkyl chains do it better. Journal of Materials Chemistry C, 2022, 10, 13815-13825.	5.5	8
103	Structural, Mechanical, and Superconducting Properties of Clathrates. Carbon Materials, 2010, , 171-206.	1.2	7
104	Optical properties of graphene quantum dots: the role of chiral symmetry. 2D Materials, 2020, 7, 025041.	4.4	6
105	Superconductivity in doped clathrates, diamond and silicon. Comptes Rendus Physique, 2011, 12, 584-590.	0.9	4
106	Size-dependent optical absorption of Cu2ZnSn(Se,S)4 quantum dot sensitizers from ab initio many-body methods. European Physical Journal B, 2018, 91, 1.	1.5	3
107	Atomistic Tight-Binding Approaches to Quantum Transport. , 2009, , .		2
108	Electronic Properties of Boron-Nitride and Boron Carbonitride Nanotubes and Related Heterojunctions. , 2009, , 83-103.		2

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109	First-Principles Theoretical Modeling of Nanotube Growth. , 2001, , 149-170.		0
110	The Growth of Carbon and Boron Nitride Nanotubes: A Quantum Molecular Dynamics Study. Fundamental Materials Research, 2002, , 53-65.	0.1	0
111	Les semi-conducteurs supraconducteurs du groupe IV. , 2013, , 4-4.	0.1	0