Xavier Blase

List of Publications by Year
in descending order

111 papers	14,531 citations	32410 55 h-index	30277 107 g-index
112 all docs	112 docs citations	112 times ranked	14127 citing authors

#	Article	IF	Citations
1	Dopingâ€Induced Dielectric Catastrophe Prompts Freeâ€Carrier Release in Organic Semiconductors. Advanced Materials, 2022, 34, e2105376.	11.1	9
2	Doping of semicrystalline conjugated polymers: dopants within alkyl chains do it better. Journal of Materials Chemistry C, 2022, 10, 13815-13825.	2.7	8
3	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, .	0.9	9
4	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
5	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
6	Cubic-Scaling All-Electron GW Calculations with a Separable Density-Fitting Spaceâ€“Time Approach. Journal of Chemical Theory and Computation, 2021, 17, 2383-2393.	2.3	50
7	Reference Energies for Intramolecular Charge-Transfer Excitations. Journal of Chemical Theory and Computation, 2021, 17, 3666-3686.	2.3	51
8	Photoluminescent properties of the carbon-dimer defect in hexagonal boron-nitride: A many-body finite-size cluster approach. Physical Review Materials, 2021, 5, .	0.9	16
9	Dynamical correction to the Betheâ€“Salpeter equation beyond the plasmon-pole approximation. Journal of Chemical Physics, 2020, 153, 114120.	1.2	21
10	The Betheâ€“Salpeter Equation Formalism: From Physics to Chemistry. Journal of Physical Chemistry Letters, 2020, 11, 7371-7382.	2.1	96
11	Orientation dependent molecular electrostatics drives efficient charge generation in homojunction organic solar cells. Nature Communications, 2020, 11, 4617.	5.8	60
12	Robust Analytic-Continuation Approach to Many-Body GW Calculations. Journal of Chemical Theory and Computation, 2020, 16, 1742-1756.	2.3	47
13	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.	2.3	10
14	Optical properties of graphene quantum dots: the role of chiral symmetry. 2D Materials, 2020, 7, 025041.	2.0	6
15	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></mm 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> Physical Review B, 2020, 101, .	1.1	31
16	Pros and Cons of the Betheâ€“Salpeter Formalism for Ground-State Energies. Journal of Physical Chemistry Letters, 2020, 11, 3536-3545.	2.1	23
17	Ground-state correlation energy of beryllium dimer by the Bethe-Salpeter equation. SciPost Physics, 2020, 8, .	1.5	12
18	Separable resolution-of-the-identity with all-electron Gaussian bases: Application to cubic-scaling RPA. Journal of Chemical Physics, 2019, 150, 174120.	1.2	43

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19	Host dependence of the electron affinity of molecular dopants. Materials Horizons, 2019, 6, 107-114.	6.4	64
20	The Betheâ€“Salpeter formalism with polarisable continuum embedding: reconciling linear-response and state-specific features. Chemical Science, 2018, 9, 4430-4443.	3.7	55
21	Accurate description of charged excitations in molecular solids from embedded many-body perturbation theory. Physical Review B, 2018, 97, .	1.1	46
22	The Betheâ€“Salpeter equation in chemistry: relations with TD-DFT, applications and challenges. Chemical Society Reviews, 2018, 47, 1022-1043.	18.7	158
23	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.	0.6	3
24	Bethe-Salpeter study of cationic dyes: Comparisons with ADC(2) and TD-DFT. Journal of Chemical Physics, 2017, 146, 034301.	1.2	21
25	Benchmark of Bethe-Salpeter for Triplet Excited-States. Journal of Chemical Theory and Computation, 2017, 13, 767-783.	2.3	65
26	Hybrid and Constrained Resolution-of-Identity Techniques for Coulomb Integrals. Journal of Chemical Theory and Computation, 2017, 13, 1199-1208.	2.3	25
27	Modeling the Photochromeâ€“TiO₂ Interface with Betheâ€“Salpeter and Time-Dependent Density Functional Theory Methods. Journal of Physical Chemistry Letters, 2017, 8, 936-940.	2.1	19
28	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.	2.1	78
29	Tuning Optical Properties of Dibenzochrysenes by Functionalization: A Many-Body Perturbation Theory Study. Journal of Physical Chemistry C, 2017, 121, 24480-24488.	1.5	18
30	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.	2.9	22
31	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.	1.1	21
32	Correlated electron-hole mechanism for molecular doping in organic semiconductors. Physical Review Materials, 2017, 1, .	0.9	42
33	GW and Bethe-Salpeter study of small water clusters. Journal of Chemical Physics, 2016, 144, 034109.	1.2	38
34	Combining the GW formalism with the polarizable continuum model: A state-specific non-equilibrium approach. Journal of Chemical Physics, 2016, 144, 164106.	1.2	46
35	Assessment of the Accuracy of the Betheâ€“Salpeter (BSE/GW) Oscillator Strengths. Journal of Chemical Theory and Computation, 2016, 12, 3969-3981.	2.3	44
36	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.	2.1	70

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37	Assessment of the convergence of partially self-consistent BSE/GW calculations. Molecular Physics, 2016, 114, 957-967.	0.8	19
38	Does Excess Energy Assist Photogeneration in an Organic Lowâ€Bandgap Solar Cell?. Advanced Functional Materials, 2015, 25, 1287-1295.	7.8	31
39	First Principles Calculations of Charge Transfer Excitations in Polymerâ€“Fullerene Complexes: Influence of Excess Energy. Advanced Functional Materials, 2015, 25, 1972-1984.	7.8	59
40	Benchmarking the Betheâ€“Salpeter Formalism on a Standard Organic Molecular Set. Journal of Chemical Theory and Computation, 2015, 11, 3290-3304.	2.3	172
41	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.	2.3	208
42	Ab Initio Calculations of Open-Cell Voltage in Li-Ion Organic Radical Batteries. Journal of Physical Chemistry C, 2015, 119, 23373-23378.	1.5	31
43	Benchmark Many-Body GW and Betheâ€“Salpeter Calculations for Small Transition Metal Molecules. Journal of Chemical Theory and Computation, 2014, 10, 3934-3943.	2.3	98
44	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.	2.3	34
45	Fast and Accurate Electronic Excitations in Cyanines with the Many-Body Betheâ€“Salpeter Approach. Journal of Chemical Theory and Computation, 2014, 10, 1212-1218.	2.3	88
46	Resonant hot charge-transfer excitations in fullerene-porphyrin complexes: Many-body Bethe-Salpeter study. Physical Review B, 2013, 87, .	1.1	46
47	Giant osmotic energy conversion measured in a single transmembrane boron nitride nanotube. Nature, 2013, 494, 455-458.	13.7	937
48	Les semi-conducteurs supraconducteurs du groupe IV. , 2013, , 4-4.	0.1	0
49	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
50	Short-Range to Long-Range Charge-Transfer Excitations in the Zincbacteriochlorin-Bacteriochlorin Complex: A Bethe-Salpeter Study. Physical Review Letters, 2012, 109, 167801.	2.9	97
51	Many-body Green's function study of coumarins for dye-sensitized solar cells. Physical Review B, 2012, 86, .	1.1	51
52	Molecular Fingerprints in the Electronic Properties of Crystalline Organic Semiconductors: From Experiment to Theory. Physical Review Letters, 2012, 108, 256401.	2.9	57
53	Charge-transfer excitations in molecular donor-acceptor complexes within the many-body Bethe-Salpeter approach. Applied Physics Letters, 2011, 99, .	1.5	142
54	Superconductivity in doped clathrates, diamond and silicon. Comptes Rendus Physique, 2011, 12, 584-590.	0.3	4

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55	Quantum transport properties of chemically functionalized long semiconducting carbon nanotubes. Nano Research, 2010, 3, 288-295.	5.8	48
56	Boron-nitride and boron-carbonitride nanotubes: synthesis, characterization and theory. Advances in Physics, 2010, 59, 101-179.	35.9	143
57	Structural, Mechanical, and Superconducting Properties of Clathrates. Carbon Materials, 2010, , 171-206.	0.2	7
58	Superconducting group-IV semiconductors. Nature Materials, 2009, 8, 375-382.	13.3	161
59	Carbon nanotube chemistry and assembly for electronic devices. Comptes Rendus Physique, 2009, 10, 330-347.	0.3	28
60	Chemically Induced Mobility Gaps in Graphene Nanoribbons: A Route for Upscaling Device Performances. Nano Letters, 2009, 9, 2725-2729.	4.5	120
61	Effect of the Chemical Functionalization on Charge Transport in Carbon Nanotubes at the Mesoscopic Scale. Nano Letters, 2009, 9, 940-944.	4.5	118
62	Atomistic Tight-Binding Approaches to Quantum Transport. , 2009, , .		2
63	Electronic Properties of Boron-Nitride and Boron Carbonitride Nanotubes and Related Heterojunctions. , 2009, , 83-103.		2
64	Thermal Stability of Graphene and Nanotube Covalent Functionalization. Nano Letters, 2008, 8, 3315-3319.	4.5	91
65	LOW-DIMENSIONAL QUANTUM TRANSPORT PROPERTIES OF CHEMICALLY-DISORDERED CARBON NANOTUBES: FROM WEAK TO STRONG LOCALIZATION REGIMES. Modern Physics Letters B, 2007, 21, 1955-1982.	1.0	65
66	Superconductivity in doped cubic silicon: An ab initio study. Applied Physics Letters, 2007, 90, 142511.	1.5	36
67	Electronic and transport properties of nanotubes. Reviews of Modern Physics, 2007, 79, 677-732.	16.4	1,234
68	Conductance, Surface Traps, and Passivation in Doped Silicon Nanowires. Nano Letters, 2006, 6, 2674-2678.	4.5	100
69	Surface Segregation and Backscattering in Doped Silicon Nanowires. Physical Review Letters, 2006, 96, 166805.	2.9	166
70	Superconductivity in doped cubic silicon. Nature, 2006, 444, 465-468.	13.7	238
71	High pressure synthesis and properties of intercalated silicon clathrates. Journal of Physics and Chemistry of Solids, 2006, 67, 1117-1121.	1.9	35
72	An analytical model for the thermal conductivity of silicon nanostructures. Journal of Applied Physics, 2005, 97, 104318.	1.1	82

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73	Exceptional Ideal Strength of Carbon Clathrates. Physical Review Letters, 2004, 92, 215505.	2.9	107
74	Guest displacement in silicon clathrates. Physical Review B, 2004, 69, .	1.1	36
75	First principles study of gold adsorption and diffusion on graphite. Surface Science, 2004, 564, 173-178.	0.8	63
76	Role of the Dopant in the Superconductivity of Diamond. Physical Review Letters, 2004, 93, 237004.	2.9	164
77	Superconductivity in Dopedsp3Semiconductors: The Case of the Clathrates. Physical Review Letters, 2003, 91, 247001.	2.9	136
78	GWstudy of the metal-insulator transition of bcc hydrogen. Physical Review B, 2002, 66, .	1.1	35
79	N-doping and coalescence of carbon nanotubes: synthesis and electronic properties. Applied Physics A: Materials Science and Processing, 2002, 74, 355-361.	1.1	392
80	The Growth of Carbon and Boron Nitride Nanotubes: A Quantum Molecular Dynamics Study. Fundamental Materials Research, 2002, , 53-65.	0.1	0
81	Identification of Electron Donor States in N-Doped Carbon Nanotubes. Nano Letters, 2001, 1, 457-460.	4.5	727
82	Quasiparticle band structure of lanthanum hydride. Physical Review B, 2001, 64, .	1.1	14
83	Quasiparticle Effects on Tunneling Currents: A Study ofC2H4Adsorbed on theSi(001)-(2Ã—1)Surface. Physical Review Letters, 2001, 86, 2110-2113.	2.9	41
84	Tailoring Band Gap and Hardness by Intercalation: Anab initioStudy ofI8@Siâˆ'46and Related Doped Clathrates. Physical Review Letters, 2001, 87, 206405.	2.9	64
85	First-Principles Theoretical Modeling of Nanotube Growth. , 2001, , 149-170.		0
86	Properties of composite BxCyNz nanotubes and related heterojunctions. Computational Materials Science, 2000, 17, 107-114.	1.4	46
87	Structure and Energy of the90Â°Partial Dislocation in Diamond: A CombinedAb Initioand Elasticity Theory Analysis. Physical Review Letters, 2000, 84, 5780-5783.	2.9	75
88	Photolysis experiments on SiC mixed clusters: From silicon carbide clusters to silicon-doped fullerenes. Journal of Chemical Physics, 1999, 110, 6927-6938.	1.2	102
89	Boron-Mediated Growth of Long Helicity-Selected Carbon Nanotubes. Physical Review Letters, 1999, 83, 5078-5081.	2.9	119
90	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.	1.1	132

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91	High Pressure Behavior of Silicon Clathrates: A New Class of Low Compressibility Materials. Physical Review Letters, 1999, 83, 5290-5293.	2.9	146
92	Synthesis and Structure of Silicon-doped Heterofullerenes. Physical Review Letters, 1998, 80, 5365-5368.	2.9	163
93	Effects of Nanodomain Formation on the Electronic Structure of Doped Carbon Nanotubes. Physical Review Letters, 1998, 81, 2332-2335.	2.9	305
94	Electronic signature of the pentagonal rings in silicon clathrate phases: Comparison with cluster-assembled films. Physical Review B, 1998, 58, 12590-12593.	1.1	35
95	Frustration Effects and Microscopic Growth Mechanisms for BN Nanotubes. Physical Review Letters, 1998, 80, 1666-1669.	2.9	163
96	Theory of composite BxCyNz nanotube heterojunctions. Applied Physics Letters, 1997, 70, 197-199.	1.5	243
97	Theoretical Models for the Optical Properties of Clusters and Nanostructures. International Journal of Modern Physics B, 1997, 11, 2727-2776.	1.0	25
98	Electronic Structure and Localized States at Carbon Nanotube Tips. Physical Review Letters, 1997, 78, 2811-2814.	2.9	355
99	Microscopic Growth Mechanisms for Carbon Nanotubes. Science, 1997, 275, 647-649.	6.0	220
100	Theoretical study of one-dimensional chains of metal atoms in nanotubes. Physical Review B, 1996, 53, 4023-4026.	1.1	93
101	Ab InitioPhotoabsorption Spectra and Structures of Small Semiconductor and Metal Clusters. Physical Review Letters, 1996, 77, 247-250.	2.9	193
102	Mixed-space formalism for the dielectric response in periodic systems. Physical Review B, 1995, 52, R2225-R2228.	1.1	37
103	Synthesis ofBxCyNznanotubules. Physical Review B, 1995, 51, 11229-11232.	1.1	413
104	Anharmonicity and Lifetime of the CH Stretch Mode on Diamond H/C(111)-(1 Ã— 1). Europhysics Letters, 1995, 30, 399-404.	0.7	62
105	Quasiparticle band structure of bulk hexagonal boron nitride and related systems. Physical Review B, 1995, 51, 6868-6875.	1.1	583
106	Ionic Cohesion and Electron Doping of Thin Carbon Tubules with Alkali Atoms. Physical Review Letters, 1995, 74, 2993-2996.	2.9	163
107	Self-energy effects on the surface-state energies of H-Si(111)1Ã—1. Physical Review B, 1994, 49, 4973-4980.	1.1	89
108	Stability and Band Gap Constancy of Boron Nitride Nanotubes. Europhysics Letters, 1994, 28, 335-340.	0.7	1,406

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109	Hybridization effects and metallicity in small radius carbon nanotubes. Physical Review Letters, 1994, 72, 1878-1881.	2.9	931
110	Quasiparticle band structures of six II-VI compounds: ZnS, ZnSe, ZnTe, CdS, CdSe, and CdTe. Physical Review B, 1994, 50, 10780-10787.	1.1	366
111	Electronic structure and its dependence on local order for H/Si(111)-(1Ã—1) surfaces. Physical Review Letters, 1993, 70, 1992-1995.	2.9	153