Silvana Botti

List of Publications by Year
in descending order

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130 papers	6,960 citations	81743 39 h-index	62479 80 g-index
140 all docs	140 docs citations	140 times ranked	8011 citing authors

#	Article	IF	Citations
1	Recent advances and applications of machine learning in solid-state materials science. Npj Computational Materials, 2019, 5, .	3.5	1,289
2	Density-based mixing parameter for hybrid functionals. Physical Review B, 2011, 83, .	1.1	338
3	Crystal Structure of Cold Compressed Graphite. Physical Review Letters, 2012, 108, 065501.	2.9	292
4	Stability and electronic properties of new inorganic perovskites from high-throughput ab initio calculations. Journal of Materials Chemistry C, 2016, 4, 3157-3167.	2.7	235
5	Direct-bandgap emission from hexagonal Ge and SiGe alloys. Nature, 2020, 580, 205-209.	13.7	231
6	Predicting the Thermodynamic Stability of Solids Combining Density Functional Theory and Machine Learning. Chemistry of Materials, 2017, 29, 5090-5103.	3.2	217
7	Time-dependent density-functional theory for extended systems. Reports on Progress in Physics, 2007, 70, 357-407.	8.1	201
8	Long-range contribution to the exchange-correlation kernel of time-dependent density functional theory. Physical Review B, 2004, 69, .	1.1	184
9	Origin of the Optical Contrast in Phase-Change Materials. Physical Review Letters, 2007, 98, 236403.	2.9	162
10	Exchange-correlation functionals for band gaps of solids: benchmark, reparametrization and machine learning. Npj Computational Materials, 2020, 6, .	3.5	156
11	Large-Scale Benchmark of Exchangeâ€“Correlation Functionals for the Determination of Electronic Band Gaps of Solids. Journal of Chemical Theory and Computation, 2019, 15, 5069-5079.	2.3	151
12	Low-energy silicon allotropes with strong absorption in the visible for photovoltaic applications. Physical Review B, 2012, 86, .	1.1	138
13	Strong Interplay between Structure and Electronic Properties in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>CuIn</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mi) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 262 Td (mathvariant="bold">S</mml:mi><mml:m Physical Review Letters, 2010, 104, 056401.	2.9	133
14	Band structures of Cu2ZnSnS4 and Cu2ZnSnSe4 from many-body methods. Applied Physics Letters, 2011, 98, 241915.	1.5	112
15	Time-dependent density functional theory scheme for efficient calculations of dynamic (hyper)polarizabilities. Journal of Chemical Physics, 2007, 126, 184106.	1.2	106
16	Prediction of Stable Nitride Perovskites. Chemistry of Materials, 2015, 27, 5957-5963.	3.2	102
17	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
18	Effects of Electronic and Lattice Polarization on the Band Structure of Delafossite Transparent Conductive Oxides. Physical Review Letters, 2010, 104, 136401.	2.9	88

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19	High-Pressure Structures of Disilane and Their Superconducting Properties. Physical Review Letters, 2012, 108, 117004.	2.9	86
20	First-principles study of the band structure and optical absorption of CuGaS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2011, 84, .	1.1	74
21	Low-density silicon allotropes for photovoltaic applications. Physical Review B, 2015, 92, .	1.1	70
22	Roadmap on Machine learning in electronic structure. Electronic Structure, 2022, 4, 023004.	1.0	69
23	TDDFT from molecules to solids: The role of long-range interactions. International Journal of Quantum Chemistry, 2005, 102, 684-701.	1.0	65
24	Band structures of delafossite transparent conductive oxides from a self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>approach. Physical Review B, 2010, 82, .	1.1	63
25	Sodiumâ€“gold binaries: novel structures for ionic compounds from anab initiostructural search. New Journal of Physics, 2013, 15, 115007.	1.2	58
26	Strong Renormalization of the Electronic Band Gap due to Lattice Polarization in 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>Formalism. Physical Review Letters, 2013, 110, 226404.	2.9	56
27	Identification of Novel Cu, Ag, and Au Ternary Oxides from Global Structural Prediction. Chemistry of Materials, 2015, 27, 4562-4573.	3.2	56
28	Estimating Excitonic Effects in the Absorption Spectra of Solids: Problems and Insight from a Guided Iteration Scheme. Physical Review Letters, 2015, 114, 146402.	2.9	56
29	Energy dependence of the exchange-correlation kernel of time-dependent density functional theory: A simple model for solids. Physical Review B, 2005, 72, .	1.1	54
30	First-Principles Identification of Single Photon Emitters Based on Carbon Clusters in Hexagonal Boron Nitride. Journal of Physical Chemistry A, 2021, 125, 1325-1335.	1.1	51
31	Optical and magnetic properties of boron fullerenes. Physical Chemistry Chemical Physics, 2009, 11, 4523.	1.3	50
32	Identification of fullerene-like CdSe nanoparticles from optical spectroscopy calculations. Physical Review B, 2007, 75, .	1.1	47
33	The planar-to-tubular structural transition in boron clusters from optical absorption. Journal of Chemical Physics, 2005, 123, 014310.	1.2	46
34	High-throughput search of ternary chalcogenides for p-type transparent electrodes. Scientific Reports, 2017, 7, 43179.	1.6	46
35	Comment on â€œQuantum Confinement and Electronic Properties of Silicon Nanowiresâ€. Physical Review Letters, 2005, 94, 219701; author reply 219702.	2.9	43
36	Novel Structural Motifs in Low Energy Phases of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>LiAlH</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 108, 205505.	2.9	43

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37	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
38	Local Modified Becke-Johnson Exchange-Correlation Potential for Interfaces, Surfaces, and Two-Dimensional Materials. Journal of Chemical Theory and Computation, 2020, 16, 2654-2660.	2.3	42
39	From mesoscale to nanoscale mechanics in single-wall carbon nanotubes. Carbon, 2017, 123, 145-150.	5.4	41
40	Predicting stable crystalline compounds using chemical similarity. Npj Computational Materials, 2021, 7, .	3.5	41
41	Accurate electronic and optical properties of hexagonal germanium for optoelectronic applications. Physical Review Materials, 2019, 3, .	0.9	41
42	Conducting Boron Sheets Formed by the Reconstruction of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Boron (111) Surface. Physical Review Letters, 2013, 111, 136101.	2.9	40
43	Density-functional tight-binding study of the collapse of carbon nanotubes under hydrostatic pressure. Carbon, 2014, 69, 355-360.	5.4	40
44	Stable hybrid organicâ€“inorganic halide perovskites for photovoltaics from ab initio high-throughput calculations. Journal of Materials Chemistry A, 2018, 6, 6463-6475.	5.2	40
45	Low-Energy Polymeric Phases of Alanates. Physical Review Letters, 2013, 110, 135502.	2.9	38
46	Crystal graph attention networks for the prediction of stable materials. Science Advances, 2021, 7, eabi7948.	4.7	37
47	Ab InitioCalculations of the Anisotropic Dielectric Tensor ofGaAs/AlAsSuperlattices. Physical Review Letters, 2002, 89, 216803.	2.9	35
48	Computational acceleration of prospective dopant discovery in cuprous iodide. Physical Chemistry Chemical Physics, 2019, 21, 18839-18849.	1.3	34
49	Mechanism of surface passivation of methylammonium lead tribromide single crystals by benzylamine. Applied Physics Reviews, 2019, 6, 031401.	5.5	34
50	Carbon structures and defect planes in diamond at high pressure. Physical Review B, 2013, 88, .	1.1	32
51	Double perovskites as p-type conducting transparent semiconductors: a high-throughput search. Journal of Materials Chemistry A, 2019, 7, 14705-14711.	5.2	32
52	Efficient calculation of van der Waals dispersion coefficients with time-dependent density functional theory in real time: Application to polycyclic aromatic hydrocarbons. Journal of Chemical Physics, 2007, 127, 014107.	1.2	31
53	Predicting the stability of ternary intermetallics with density functional theory and machine learning. Journal of Chemical Physics, 2018, 148, 241728.	1.2	30
54	Out-of-plane excitons in two-dimensional crystals. Physical Review B, 2019, 99, .	1.1	30

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55	Feedback mechanism for the stability of the band gap of CuInSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	1.1	29
56	Raman activity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:mrow allotropes under pressure: A density functional theory study. Physical Review B, 2012, 85, .	1.1	28
57	Radial collapse of carbon nanotubes for conductivity optimized polymer composites. Carbon, 2016, 106, 64-73.	5.4	28
58	Pressure-induced radial collapse in few-wall carbon nanotubes: A combined theoretical and experimental study. Carbon, 2017, 125, 429-436.	5.4	27
59	Cluster-surface and cluster-cluster interactions:Ab initiocalculations and modeling of asymptotic van der Waals forces. Physical Review B, 2008, 78, .	1.1	26
60	Bandgap of two-dimensional materials: Thorough assessment of modern exchangeâ€“correlation functionals. Journal of Chemical Physics, 2021, 155, 104103.	1.2	26
61	First-principles predicted low-energy structures of NaSc(BH4)4. Journal of Chemical Physics, 2014, 140, 124708.	1.2	25
62	Materials Design On-the-Fly. Journal of Chemical Theory and Computation, 2015, 11, 3955-3960.	2.3	25
63	The ground state of two-dimensional silicon. 2D Materials, 2018, 5, 035010.	2.0	25
64	Rare-earth magnetic nitride perovskites. JPhys Materials, 2019, 2, 025003.	1.8	25
65	Validation of Pseudopotential Calculations for the Electronic Band Gap of Solids. Journal of Chemical Theory and Computation, 2020, 16, 3620-3627.	2.3	25
66	Ab initioand semiempirical dielectric response of superlattices. Physical Review B, 2004, 70, .	1.1	24
67	Excitonic effects in the optical properties of CdSe nanowires. Applied Physics Letters, 2010, 96, .	1.5	24
68	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 the Bethe-Salpeter equation. Physical Review B, 2015, 91, .	1.1	24
69	Growth dynamics of hydrogenated silicon nanoparticles under realistic conditions of a plasma reactor. Computational Materials Science, 2006, 35, 216-222.	1.4	21
70	Superconductivity in layered binary silicides: A density functional theory study. Physical Review B, 2011, 84, .	1.1	21
71	Optimized Exchange and Correlation Semilocal Functional for the Calculation of Energies of Formation. Journal of Chemical Theory and Computation, 2015, 11, 3844-3850.	2.3	21
72	Novel crystal structures for lithiumâ€“silicon alloy predicted by minima hopping method. Journal of Alloys and Compounds, 2016, 655, 147-154.	2.8	21

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73	Local Hybrid Density Functional for Interfaces. Journal of Chemical Theory and Computation, 2018, 14, 939-947.	2.3	21
74	Accurate electronic band gaps of two-dimensional materials from the local modified Becke-Johnson potential. Physical Review B, 2020, 101, .	1.1	21
75	Atomic and electronic properties of quasi-one-dimensional MoS₂ nanowires. Journal of Materials Research, 2013, 28, 240-249.	1.2	20
76	Structural prediction of two-dimensional materials under strain. 2D Materials, 2017, 4, 045009.	2.0	19
77	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>Doping in Expanded Phases of ZnO: AnAbÂInitioStudy. Physical Review Letters, 2012, 108, 115903.	2.9	18
78	Anisotropic layered Bi2Te3-In2Te3 composites: control of interface density for tuning of thermoelectric properties. Scientific Reports, 2017, 7, 43611.	1.6	18
79	A high-throughput study of oxynitride, oxyfluoride and nitrofluoride perovskites. Journal of Materials Chemistry A, 2021, 9, 8501-8513.	5.2	18
80	Local atomic order and optical properties in amorphous and laser-crystallized GeTe. Comptes Rendus Physique, 2009, 10, 514-527.	0.3	17
81	Enhancing the Superconducting Transition Temperature of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BaSi</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>by Structural Tuning. Physical Review Letters, 2011, 106, 087002.	2.9	17
82	Stable Ordered Phases of Cuprous Iodide with Complexes of Copper Vacancies. Chemistry of Materials, 2019, 31, 7877-7882.	3.2	17
83	Nitrogen-hydrogen-oxygen ternary phase diagram: New phases at high pressure from structural prediction. Physical Review Materials, 2018, 2, .	0.9	17
84	Nanostructured water and carbon dioxide inside collapsing carbon nanotubes at high pressure. Physical Chemistry Chemical Physics, 2016, 18, 19926-19932.	1.3	16
85	Thermodynamic, electronic, and optical properties of graphene oxide: A statisticalab initioapproach. Physical Review B, 2017, 95, .	1.1	16
86	Efficient strain-induced light emission in lonsdaleite germanium. Physical Review Materials, 2021, 5, .	0.9	16
87	Prediction and Synthesis of a Non-Zintl Silicon Clathrate. Chemistry of Materials, 2016, 28, 3711-3717.	3.2	15
88	Investigation of new phases in the Baâ€“Si phase diagram under high pressure using ab initio structural search. Physical Chemistry Chemical Physics, 2016, 18, 8108-8114.	1.3	15
89	Novel phases of lithium-aluminum binaries from first-principles structural search. Journal of Chemical Physics, 2015, 142, 024710.	1.2	14
90	Structural prediction of stabilized atomically thin tin layers. Npj 2D Materials and Applications, 2019, 3, .	3.9	14

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91	Prediction of a novel monoclinic carbon allotrope. European Physical Journal B, 2013, 86, 1.	0.6	13
92	Ab Initio Electronic Gaps of Ge Nanodots: The Role of Self-Energy Effects. Journal of Physical Chemistry C, 2013, 117, 14229-14234.	1.5	12
93	The crystal structure of p-type transparent conductive oxide CuBO2. MRS Communications, 2013, 3, 157-160.	0.8	12
94	Local versus global electronic properties of chalcopyrite alloys: X-ray absorption spectroscopy and ab initio calculations. Journal of Applied Physics, 2014, 116, 093703.	1.1	12
95	Topological Crystalline Insulator in a New Bi Semiconducting Phase. Scientific Reports, 2016, 6, 21790.	1.6	12
96	Research Update: Stable single-phase Zn-rich Cu2ZnSnSe4 through In doping. APL Materials, 2016, 4, 070701.	2.2	11
97	Superconducting hydrogen tubes in hafnium hydrides at high pressure. Physical Review B, 2021, 104, .	1.1	11
98	Superconductivity in an expanded phase of ZnO: anab initiostudy. New Journal of Physics, 2015, 17, 043034.	1.2	10
99	On the calculation of the bandgap of periodic solids with MGGA functionals using the total energy. Journal of Chemical Physics, 2019, 151, 161102.	1.2	10
100	Direct insight into the structure-property relation of interfaces from constrained crystal structure prediction. Nature Communications, 2021, 12, 811.	5.8	10
101	Electronic Structure of Molecules, Surfaces, and Molecules on Surfaces with the Local Modified Beckeâ€“Johnson Exchangeâ€“Correlation Potential. Journal of Chemical Theory and Computation, 2021, 17, 4746-4755.	2.3	10
102	High-pressure phases of VO2 from the combination of Raman scattering and ab initio structural search. Physical Review B, 2018, 97, .	1.1	9
103	Electronic and Optical Properties of Small Metal Fluoride Clusters. ACS Omega, 2020, 5, 13268-13277.	1.6	8
104	Novel two-dimensional siliconâ€“carbon binaries by crystal structure prediction. Physical Chemistry Chemical Physics, 2020, 22, 8442-8449.	1.3	8
105	Unveiling Planar Defects in Hexagonal Group IV Materials. Nano Letters, 2021, 21, 3619-3625.	4.5	8
106	A dataset of 175k stable and metastable materials calculated with the PBEsol and SCAN functionals. Scientific Data, 2022, 9, 64.	2.4	8
107	Structure and Optical Properties of Small (TiO₂)_n Nanoparticles, n = 21â€“24. Journal of Physical Chemistry C, 2017, 121, 9528-9536.	1.5	7
108	Layered CuI: a path to 2D p-type transparent conducting materials. Journal of Materials Chemistry C, 2021, 9, 11284-11291.	2.7	7

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109	From pseudo-direct hexagonal germanium to direct silicon-germanium alloys. Physical Review Materials, 2021, 5, .	0.9	7
110	Electronic Structure and Epitaxy of CdTe Shells on InSb Nanowires. Advanced Science, 2022, 9, e2105722.	5.6	7
111	Machine-learning correction to density-functional crystal structure optimization. MRS Bulletin, 2022, 47, 765-771.	1.7	7
112	Applications of Time-Dependent Density Functional Theory. Physica Scripta, 2004, T109, 54.	1.2	6
113	Detection of Cu2Zn5SnSe8 and Cu2Zn6SnSe9 phases in co-evaporated Cu2ZnSnSe4 thin-films. Applied Physics Letters, 2015, 107, .	1.5	6
114	RigamontietÂal.Reply:. Physical Review Letters, 2016, 117, 159702.	2.9	6
115	Chemically Tunable Properties of Graphene Covered Simultaneously with Hydroxyl and Epoxy Groups. Journal of Physical Chemistry C, 2017, 121, 27603-27611.	1.5	6
116	Alloying effects on the optical properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ge</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:mr from time-dependent density functional theory and comparison with effective-medium theory. Physical Review B, 2009, 79, .	1.1	5
117	Modeling van der Waals interactions between proteins and inorganic surfaces from time-dependent density functional theory calculations. Physical Chemistry Chemical Physics, 2011, 13, 15055.	1.3	5
118	Halogen molecular modifications at high pressure: the case of iodine. Physical Chemistry Chemical Physics, 2021, 23, 3321-3326.	1.3	5
119	Defect levels from SCAN and MBJ meta-GGA exchange-correlation potentials. Physical Review B, 2021, 104, .	1.1	5
120	Comment on â€œTopological Insulators in Ternary Compounds with a Honeycomb Latticeâ€• Physical Review Letters, 2013, 110, 129701.	2.9	4
121	A Global-Optimization Study of the Phase Diagram of Free-Standing Hydrogenated Two-Dimensional Silicon. Journal of Physical Chemistry C, 2021, 125, 6298-6305.	1.5	4
122	Point defects in hexagonal silicon. Physical Review Materials, 2021, 5, .	0.9	4
123	Giant Optical Oscillator Strengths in Perturbed Hexagonal Germanium. Physica Status Solidi - Rapid Research Letters, 0, , 2100555.	1.2	4
124	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
125	Atomic scale structure and its impact on the band gap energy for Cu₂Zn(Sn,Ge)Se₄ kesterite alloys. JPhys Energy, 2020, 2, 035004.	2.3	3
126	Superconductivity in S-rich phases of lanthanum sulfide under high pressure. Physical Review Materials, 2022, 6, .	0.9	3

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127	Comment on â€œTowards Direct-Gap Silicon Phases by the Inverse Band Structure Design Approachâ€. Physical Review Letters, 2014, 112, 199801.	2.9	2
128	Absorption mechanism of dopamine/DOPAC-modified TiO2 nanoparticles by time-dependent density functional theory calculations. Materials Today Energy, 2021, 19, 100571.	2.5	2
129	Publisher's Note: 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></mm the Bethe-Salpeter equation [Phys. Rev. B91, 075134 (2015)]. Physical Review B, 2016, 93, .	1.1	1
130	Bishop's hat silicene: a planar square silicon bilayer decorated with adatoms. Physical Chemistry Chemical Physics, 2021, 23, 16942-16947.	1.3	0