Alexandra Carvalho

List of Publications by Citations

102 papers	11,765 citations	40 h-index	105 g-index
105 ext. papers	13,699 ext. citations	7.2 avg, IF	6.89 L-index

#	Paper	IF	Citations
102	2D materials and van der Waals heterostructures. *Science*, **2016**, 353, aac9439	33.3	3469
101	Strain-induced gap modification in black phosphorus. *Physical Review Letters*, **2014**, 112, 176801	7.4	1113
100	Phosphorene: from theory to applications. *Nature Reviews Materials*, **2016**, 1,	73.3	571
99	Tunable optical properties of multilayer black phosphorus thin films. *Physical Review B*, **2014**, 90,	3.3	496
98	Oxygen defects in phosphorene. *Physical Review Letters*, **2015**, 114, 046801	7.4	432
97	Transport properties of pristine few-layer black phosphorus by van der Waals passivation in an inert atmosphere. *Nature Communications*, **2015**, 6, 6647	17.4	394
96	Origin of indirect optical transitions in few-layer MoS2, WS2, and WSe2. *Nano Letters*, **2013**, 13, 5627-34	11.5	365
95	Spin-orbit proximity effect in graphene. *Nature Communications*, **2014**, 5, 4875	17.4	321
94	Phosphorene analogues: Isoelectronic two-dimensional group-IV monochalcogenides with orthorhombic structure. *Physical Review B*, **2015**, 92,	3.3	301
93	Photocarrier relaxation pathway in two-dimensional semiconducting transition metal dichalcogenides. *Nature Communications*, **2014**, 5, 4543	17.4	294
92	Creating a Stable Oxide at the Surface of Black Phosphorus. *ACS Applied Materials & Interfaces*, **2015**, 7, 14557-62	9.5	258
91	Band nesting and the optical response of two-dimensional semiconducting transition metal dichalcogenides. *Physical Review B*, **2013**, 88,	3.3	207
90	Colossal Ultraviolet Photoresponsivity of Few-Layer Black Phosphorus. *ACS Nano*, **2015**, 9, 8070-7	16.7	175
89	Electron Doping of Ultrathin Black Phosphorus with Cu Adatoms. *Nano Letters*, **2016**, 16, 2145-51	11.5	165
88	Phosphorene oxides: Bandgap engineering of phosphorene by oxidation. *Physical Review B*, **2015**, 91,	3.3	158
87	Atomic healing of defects in transition metal dichalcogenides. *Nano Letters*, **2015**, 15, 3524-32	11.5	147
86	Evidence for Fast Interlayer Energy Transfer in MoSe2/WS2 Heterostructures. *Nano Letters*, **2016**, 16, 4087-93	11.5	145

85	Enhanced piezoelectricity and modified dielectric screening of two-dimensional group-IV monochalcogenides. *Physical Review B*, **2015**, 92,	3.3	135
84	Multiferroic Two-Dimensional Materials. *Physical Review Letters*, **2016**, 116, 206803	7.4	127
83	Phosphorene nanoribbons. *Europhysics Letters*, **2014**, 108, 47005	1.6	118
82	Atomically thin dilute magnetism in Co-doped phosphorene. *Physical Review B*, **2015**, 91,	3.3	109
81	Excitons in anisotropic two-dimensional semiconducting crystals. *Physical Review B*, **2014**, 90,	3.3	108
80	Polarization and valley switching in monolayer group-IV monochalcogenides. *Physical Review B*, **2016**, 94,	3.3	107
79	Gate-Tunable Giant Stark Effect in Few-Layer Black Phosphorus. *Nano Letters*, **2017**, 17, 1970-1977	11.5	106
78	Bandgap Engineering of Phosphorene by Laser Oxidation toward Functional 2D Materials. *ACS Nano*, **2015**, 9, 10411-21	16.7	102
77	Surface Functionalization of Black Phosphorus via Potassium toward High-Performance Complementary Devices. *Nano Letters*, **2017**, 17, 4122-4129	11.5	99
76	Unusually efficient photocurrent extraction in monolayer van der Waals heterostructure by tunnelling through discretized barriers. *Nature Communications*, **2016**, 7, 13278	17.4	96
75	A hybrid density functional study of lithium in ZnO: Stability, ionization levels, and diffusion. *Physical Review B*, **2009**, 80,	3.3	92
74	Light-Matter Interactions in Phosphorene. *Accounts of Chemical Research*, **2016**, 49, 1806-15	24.3	89
73	Valley physics in tin (II) sulfide. *Physical Review B*, **2016**, 93,	3.3	88
72	Hybrid Bilayer WSe2 -CH3 NH3 PbI3 Organolead Halide Perovskite as a High-Performance Photodetector. *Angewandte Chemie - International Edition*, **2016**, 55, 11945-9	16.4	71
71	Fluorescence Concentric Triangles: A Case of Chemical Heterogeneity in WS2 Atomic Monolayer. *Nano Letters*, **2016**, 16, 5559-67	11.5	70
70	Vacancies and oxidation of two-dimensional group-IV monochalcogenides. *Physical Review B*, **2016**, 94,	3.3	61
69	Cation-site intrinsic defects in Zn-doped CdTe. *Physical Review B*, **2010**, 81,	3.3	60
68	Strongly bound Mott-Wannier excitons in GeS and GeSe monolayers. *Physical Review B*, **2016**, 94,	3.3	59

67	Accessing valley degree of freedom in bulk Tin(II) sulfide at room temperature. *Nature Communications*, **2018**, 9, 1455	17.4	46
66	Exciton binding energies and luminescence of phosphorene under pressure. *Physical Review B*, **2015**, 91,	3.3	41
65	Hybrid Bilayer WSe2□CH3NH3PbI3 Organolead Halide Perovskite as a High-Performance Photodetector. *Angewandte Chemie*, **2016**, 128, 12124-12128	3.6	41
64	The oxygen dimer in Si: Its relationship to the light-induced degradation of Si solar cells?. *Applied Physics Letters*, **2011**, 98, 182101	3.4	41
63	Oxygen induced strong mobility modulation in few-layer black phosphorus. *2D Materials*, **2017**, 4, 021007	7.9	40
62	Oxygen Passivation Mediated Tunability of Trion and Excitons in MoS_{2}. *Physical Review Letters*, **2017**, 119, 077402	7.4	40
61	Self-interstitial in germanium. *Physical Review Letters*, **2007**, 99, 175502	7.4	39
60	Defects and oxidation resilience in InSe. *Physical Review B*, **2017**, 96,	3.3	36
59	Enhanced Photoresponse from Phosphorene-Phosphorene-Suboxide Junction Fashioned by Focused Laser Micromachining. *Advanced Materials*, **2016**, 28, 4090-6	24	35
58	Tunable van Hove singularities and correlated states in twisted monolayer–bilayer graphene. *Nature Physics*, **2021**, 17, 619-626	16.2	33
57	Microsteganography on WS Monolayers Tailored by Direct Laser Painting. *ACS Nano*, **2017**, 11, 713-720	16.7	31
56	Two-dimensional exciton properties in monolayer semiconducting phosphorus allotropes. *Physical Chemistry Chemical Physics*, **2016**, 18, 27829-27836	3.6	31
55	Donor and acceptor levels in semiconducting transition-metal dichalcogenides. *Physical Review B*, **2014**, 89,	3.3	31
54	Four-copper complexes in Si and the Cu-photoluminescence defect: A first-principles study. *Physical Review B*, **2011**, 84,	3.3	30
53	Density-functional study of small interstitial clusters in Si: Comparison with experiments. *Physical Review B*, **2005**, 72,	3.3	30
52	The Role of Oxygen Atoms on Excitons at the Edges of Monolayer WS. *Nano Letters*, **2019**, 19, 4641-4650	11.5	28
51	Resolving the Spatial Structures of Bound Hole States in Black Phosphorus. *Nano Letters*, **2017**, 17, 6935-6940	12.4	27
50	Tin-vacancy complex in germanium. *Journal of Applied Physics*, **2011**, 109, 083705	2.5	23

49	Two-dimensional square buckled Rashba lead chalcogenides. *Physical Review B*, **2017**, 96,	3.3	22
48	First-principles investigation of a bistable boron-oxygen interstitial pair in Si. *Physical Review B*, **2006**, 73,	3.3	20
47	Calculation of deep carrier traps in a divacancy in germanium crystals. *Applied Physics Letters*, **2006**, 88, 091919	3.4	20
46	Dual phases of crystalline and electronic structures in the nanocrystalline perovskite CsPbBr3. *NPG Asia Materials*, **2019**, 11,	10.3	20
45	Effect of Oxidation on the Doping of Silicon Nanocrystals with Group III and Group V Elements. *Journal of Physical Chemistry C*, **2012**, 116, 8243-8250	3.8	19
44	P-doping of Si nanoparticles: The effect of oxidation. *Physica Status Solidi (A) Applications and Materials Science*, **2012**, 209, 1847-1850	1.6	19
43	Electronic properties, doping, and defects in chlorinated silicon nanocrystals. *Physical Review B*, **2012**, 86,	3.3	18
42	Early stage donor-vacancy clusters in germanium. *Journal of Materials Science: Materials in Electronics*, **2007**, 18, 769-773	2.1	18
41	Structure Determination and Compositional Modification of Body-Centered Tetragonal PX-Phase Lead Titanate. *Chemistry of Materials*, **2011**, 23, 2529-2535	9.6	17
40	The self-interstitial in silicon and germanium. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2009**, 159-160, 112-116	3.1	17
39	Silicon and germanium nanocrystals: properties and characterization. *Beilstein Journal of Nanotechnology*, **2014**, 5, 1787-94	3	14
38	Influence of Ge content on the optical properties of X and W centers in dilute Si-Ge alloys. *Physical Review B*, **2011**, 84,	3.3	14
37	Adsorption of H, O, HO, OH and H on monolayer MoS. *Journal of Physics Condensed Matter*, **2018**, 30, 035003	1.8	12
36	Li-related defects in ZnO: Hybrid functional calculations. *Physica B: Condensed Matter*, **2009**, 404, 4797-4799	2.8	11
35	Electronic structure modification of Si nanocrystals with F4-TCNQ. *Physical Review B*, **2011**, 84,	3.3	11
34	Light induced degradation in B doped Cz-Si solar cells. *Physica Status Solidi (A) Applications and Materials Science*, **2012**, 209, 1894-1897	1.6	10
33	Intrinsic defect complexes in CdTe and ZnTe. *Thin Solid Films*, **2011**, 519, 7468-7471	2.2	10
32	Intrinsic defects in CdTe and CdZnTe alloys. *Physica B: Condensed Matter*, **2009**, 404, 5019-5021	2.8	10

31	Collective excitations in 2D materials. *Nature Reviews Physics*, **2020**, 2, 524-537	23.6	10
30	First-principles study of Fe and FeAl defects in SiGe alloys. *Physical Review B*, **2008**, 78,	3.3	9
29	Strong compensation of n-type Ge via formation of donor□vacancy complexes. *Physica B: Condensed Matter*, **2007**, 401-402, 179-183	2.8	9
28	Local-density-functional calculations of the vacancy-oxygen center in Ge. *Physical Review B*, **2007**, 75,	3.3	9
27	Ab initiocalculation of the local vibrational modes of the interstitial boron□interstitial oxygen defect in Si. *Journal of Physics Condensed Matter*, **2005**, 17, L155-L159	1.8	9
26	Adsorbate-localized states at water-covered (100) SrTiO3 surfaces. *Applied Physics Letters*, **2011**, 98, 012106	3.4	8
25	Boron doped Si nanoparticles: the effect of oxidation. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 1799-1803	1.3	7
24	Ab initio modeling of defect levels in Ge clusters and supercells. *Materials Science in Semiconductor Processing*, **2006**, 9, 477-483	4.3	7
23	Identification of the local vibrational modes of small nitrogen clusters in dilute GaAsN. *Physica B: Condensed Matter*, **2007**, 401-402, 339-342	2.8	6
22	Electronic and optical properties of low-dimensional group-IV monochalcogenides. *Journal of Applied Physics*, **2020**, 128, 121101	2.5	6
21	Charge Injection Rates in Hybrid Nanosilicon□Polythiophene Bulk Heterojunction Solar Cells. *Journal of Physical Chemistry C*, **2013**, 117, 110-115	3.8	5
20	Limits to N-Type Doping in Ge: Formation of Donor-Vacancy Complexes. *Defect and Diffusion Forum* , **2008**, 273-276, 93-98	0.7	5
19	Studies of the VO centre in Ge using first principles cluster calculations. *Materials Science in Semiconductor Processing*, **2006**, 9, 489-493	4.3	5
18	Theoretical Investigations of the Energy Levels of Defects in Germanium. *Solid State Phenomena*, **2005**, 108-109, 697-702	0.4	5
17	First-principles study of the diffusion mechanisms of the self-interstitial in germanium. *Journal of Physics Condensed Matter*, **2008**, 20, 135220	1.8	4
16	Identification of stable and metastable forms of VO2 centers in germanium. *Physica B: Condensed Matter*, **2007**, 401-402, 192-195	2.8	4
15	2D Electrolytes: Theory, Modeling, Synthesis, and Characterization. *Advanced Materials*, **2021**, 33, e2100442	14	4
14	The CuPL defect and the Cus1Cui3 complex. *Physica B: Condensed Matter*, **2012**, 407, 2967-2969	2.8	3

13	Self-interstitials and Frenkel pairs in electron-irradiated germanium. *Physica B: Condensed Matter*, **2007**, 401-402, 495-498	2.8	3
12	Rashba-like dispersion in buckled square lattices. *Physical Review B*, **2017**, 96,	3.3	2
11	Effect of the adsorption of ethylene carbonate on Si surfaces on the Li insertion behavior. *Chemical Physics Letters*, **2013**, 585, 157-161	2.5	2
10	Electronic structural details of donor□acancy complexes in Si-doped Ge and Ge-doped Si. *Thin Solid Films*, **2010**, 518, 2381-2385	2.2	2
9	Complexes of self-interstitials with oxygen atoms in germanium. *Materials Science in Semiconductor Processing*, **2008**, 11, 344-347	4.3	2
8	Density-functional theory study of interstitial iron and its complexes with B and Al in dilute SiGe alloys. *Materials Science in Semiconductor Processing*, **2008**, 11, 332-335	4.3	2
7	Density-functional theory study of Au, Ag and Cu defects in germanium. *Materials Science in Semiconductor Processing*, **2008**, 11, 340-343	4.3	2
6	Increased electronic coupling in silicon nanocrystal networks doped with F4-TCNQ. *Journal of Nanoscience and Nanotechnology*, **2013**, 13, 1035-8	1.3	1
5	Electronic and optical properties of chlorinated silicon nanoparticles. *Journal of Nanoscience and Nanotechnology*, **2013**, 13, 1039-42	1.3	1
4	Oxygen defects in irradiated germanium. *Journal of Materials Science: Materials in Electronics*, **2007**, 18, 781-786	2.1	1
3	Primary Defects in n-Type Irradiated Germanium: A First-Principles Investigation. *Solid State Phenomena*, **2007**, 131-133, 253-258	0.4	0
2	Electronic structure of Zn, Cu and Ni impurities in germanium. *Journal of Physics Condensed Matter*, **2011**, 23, 065802	1.8	
1	Ab Initio Studies of Local Vibrations of Small Self-Interstitials Aggregates in Silicon. *Solid State Phenomena*, **2005**, 108-109, 175-180	0.4	