Maurizia Palummo

List of Publications by Year
in descending order

119	5,890	134610	84171
papers	citations	34 h-index	75 g-index

123	123	123	9537
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in two-dimensional green materials for organic electronics applications. , 2022, , 391-422.		1
2	Photo-induced lattice distortion in 2H-MoTe₂ probed by time-resolved core level photoemission. Faraday Discussions, 2022, 236, 429-441.	1.6	5
3	Evidence for equilibrium exciton condensation in monolayer WTe2. Nature Physics, 2022, 18, 94-99.	6.5	55
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	Nature of Optical Excitations in Porphyrin Crystals: A Joint Experimental and Theoretical Study. Journal of Physical Chemistry Letters, 2021, 12, 869-875.	2.1	4
6	First-Principles Calculations of Exciton Radiative Lifetimes in Monolayer Graphitic Carbon Nitride Nanosheets: Implications for Photocatalysis. ACS Applied Nano Materials, 2021, 4, 1985-1993.	2.4	20
7	Spinorial formulation of the <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 -BSE equations and spin properties of excitons in two-dimensional transition metal dichalcogenides. Physical Review B, 2021, 103, .	1.1	16
8	Strong out-of-plane excitons in 2D hybrid halide double perovskites. Applied Physics Letters, 2021, 119, 051103.	1.5	15
9	Boosted Solar Light Absorbance in PdS₂/PtS₂ Vertical Heterostructures for Ultrathin Photovoltaic Devices. ACS Applied Materials & Interfaces, 2021, 13, 43615-43621.	4.0	14
10	Theoretical Aspects of Point Defects inÂSemiconductor Nanowires. , 2021, , 349-367.		0
11	Precise radiative lifetimes in bulk crystals from first principles: the case of wurtzite gallium nitride. Journal of Physics Condensed Matter, 2020, 32, 084001.	0.7	6
12	Ab initio studies of the optoelectronic structure of undoped and doped silicon nanocrystals and nanowires: the role of size, passivation, symmetry and phase. Faraday Discussions, 2020, 222, 217-239.	1.6	5
13	Optical Properties of Lead-Free Double Perovskites by Ab Initio Excited-State Methods. ACS Energy Letters, 2020, 5, 457-463.	8.8	64
14	Halide Pb-Free Doubleâ€“Perovskites: Ternary vs. Quaternary Stoichiometry. Energies, 2020, 13, 3516.	1.6	10
15	Close-Packed Arrangements of Flat-On Free-Base Porphyrins Driven by van der Waals Epitaxy. Crystal Growth and Design, 2020, 20, 7450-7459.	1.4	4
16	Interlayer Bound Wannier Excitons in Germanium Sulfide. Materials, 2020, 13, 3568.	1.3	3
17	A Scalable Method for Thickness and Lateral Engineering of 2D Materials. ACS Nano, 2020, 14, 4861-4870.	7.3	14
18	A monolayer transition-metal dichalcogenide as a topological excitonic insulator. Nature Nanotechnology, 2020, 15, 367-372.	15.6	61

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19	Impact of Impurities on the Electrical Conduction of Anisotropic Two-Dimensional Materials. Physical Review Applied, 2020, 13, .	1.5	16
20	Ab Initio Theory of Interband Transitions. Springer Handbooks, 2020, , 585-622.	0.3	1
21	Spatially indirect excitons in black and blue phosphorene double layers. Physical Review Materials, 2020, 4, .	0.9	6
22	Strain-induced effects on the electronic properties of 2D materials. Nanomaterials and Nanotechnology, 2020, 10, 184798042090256.	1.2	38
23	Ab initio calculations of exciton radiative lifetimes in bulk crystals, nanostructures, and molecules. Physical Review B, 2019, 100, .	1.1	30
24	Tailoring the optical properties of MoS₂ and WS₂ single layers via organic functionalization. Journal of Physics Condensed Matter, 2019, 31, 235701.	0.7	8
25	First-Principles Nonequilibrium Greenâ€™s Function Approach to Ultrafast Charge Migration in Glycine. Journal of Chemical Theory and Computation, 2019, 15, 4526-4534.	2.3	17
26	A route for minimizing emissions: sun-mediated processes and clean batteries. Current Opinion in Green and Sustainable Chemistry, 2019, 17, A1-A4.	3.2	1
27	Iceâ€Assisted Synthesis of Black Phosphorus Nanosheets as a Metalâ€Free Photocatalyst: 2D/2D Heterostructure for Broadband H₂ Evolution. Advanced Functional Materials, 2019, 29, 1902486.	7.8	116
28	Out-of-plane excitons in two-dimensional crystals. Physical Review B, 2019, 99, .	1.1	30
29	Many-body perturbation theory calculations using the yambo code. Journal of Physics Condensed Matter, 2019, 31, 325902.	0.7	269
30	Second-harmonic generation in single-layer monochalcogenides: A response from first-principles real-time simulations. Physical Review Materials, 2019, 3, .	0.9	23
31	Nature of the Electronic and Optical Excitations of Ruddlesdenâ€“Popper Hybrid Organicâ€“Inorganic Perovskites: The Role of the Many-Body Interactions. Journal of Physical Chemistry Letters, 2018, 9, 5891-5896.	2.1	51
32	Two-dimensional optical excitations in the mixed-valence Cs₂Au₂I₆ fully inorganic double perovskite. Journal of Materials Chemistry C, 2018, 6, 10197-10201.	2.7	32
33	Theory and Ab Initio Computation of the Anisotropic Light Emission in Monolayer Transition Metal Dichalcogenides. Nano Letters, 2018, 18, 3839-3843.	4.5	37
34	Optical and Electronic Properties of Two-Dimensional Layered Materials. Nanophotonics, 2017, 6, 479-493.	2.9	145
35	Role of Quantum-Confinement in Anatase Nanosheets. Journal of Physical Chemistry Letters, 2017, 8, 3867-3873.	2.1	19
36	Optical Emission in Hexagonal SiGe Nanowires. Nano Letters, 2017, 17, 4753-4758.	4.5	51

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37	Crystal Phase Effects in Si Nanowire Polytypes and Their Homojunctions. Nano Letters, 2016, 16, 5694-5700.	4.5	38
38	Temperature-dependent excitonic effects in the optical properties of single-layer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mm Physical Review B, 2016, 93, .	1.1	91
39	Electronic and Optical Properties of Oxides Nanostructures by First-Principles Approaches. , 2016, , 1071-1084.		0
40	Early oxidation stages of the strained Ge/Si(105) surface: A reflectance anisotropy spectroscopy study. Physica Status Solidi (B): Basic Research, 2015, 252, 87-94.	0.7	1
41	Electronic and Optical Properties of Oxides Nanostructures by First-Principles Approaches. , 2015, , 1-15.		0
42	Exciton Radiative Lifetimes in Two-Dimensional Transition Metal Dichalcogenides. Nano Letters, 2015, 15, 2794-2800.	4.5	517
43	Ab initio energy loss spectra of Si and Ge nanowires. Physical Chemistry Chemical Physics, 2015, 17, 29085-29089.	1.3	3
44	Understanding doping at the nanoscale: the case of codoped Si and Ge nanowires. Journal Physics D: Applied Physics, 2014, 47, 394013.	1.3	7
45	Organic Electronics: Stable Alignment of Tautomers at Room Temperature in Porphyrin 2D Layers (Adv.) Tj ETQq1 1 0.784314 rgBT /O	7.8	4
46	Electronic and optical properties of pure and modified diamondoids studied by many-body perturbation theory and time-dependent density functional theory. Journal of Chemical Physics, 2014, 141, 064308.	1.2	28
47	Stable Alignment of Tautomers at Room Temperature in Porphyrin 2D Layers. Advanced Functional Materials, 2014, 24, 958-963.	7.8	51
48	Siliconâ€“Germanium Nanowires: Chemistry and Physics in Play, from Basic Principles to Advanced Applications. Chemical Reviews, 2014, 114, 1371-1412.	23.0	151
49	Probing Two-Dimensional vs Three-Dimensional Molecular Aggregation in Metal-Free Tetraphenylporphyrin Thin Films by Optical Anisotropy. Journal of Physical Chemistry C, 2014, 118, 15649-15655.	1.5	23
50	Intermixing and buried interfacial structure in strained Ge/Si(105) facets. Physical Review B, 2013, 88, .	1.1	16
51	Correlation effects in the optical spectra of porphyrin oligomer chains: Exciton confinement and length dependence. Journal of Chemical Physics, 2013, 138, 024312.	1.2	31
52	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
53	Extraordinary Sunlight Absorption and One Nanometer Thick Photovoltaics Using Two-Dimensional Monolayer Materials. Nano Letters, 2013, 13, 3664-3670.	4.5	1,681
54	Semiconducting Monolayer Materials as a Tunable Platform for Excitonic Solar Cells. ACS Nano, 2012, 6, 10082-10089.	7.3	145

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55	The Nature of Radiative Transitions in TiO2-Based Nanosheets. Journal of Physical Chemistry C, 2012, 116, 18495-18503.	1.5	31
56	Optical absorption modulation by selective codoping of SiGe core-shell nanowires. Journal of Applied Physics, 2012, 112, .	1.1	11
57	Optical properties of the longâ€range Si(110)â€(16â€‰Ã—â€‰2) reconstruction from first principles. Physica Status Solidi (B): Basic Research, 2012, 249, 1148-1154.	0.7	8
58	Optoelectronic Properties in Monolayers of Hybridized Graphene and Hexagonal Boron Nitride. Physical Review Letters, 2012, 108, 226805.	2.9	108
59	Band structure analysis in SiGe nanowires. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2012, 177, 705-711.	1.7	13
60	Excitons at the (001) surface of anatase: Spatial behavior and optical signatures. Physical Review B, 2011, 84, .	1.1	23
61	Coexistence of Negatively and Positively Buckled Isomers onn+-DopedSi(111)â˜2Ã—1. Physical Review Letters, 2011, 106, 067601.	2.9	27
62	Silicon and Germanium Nanostructures for Photovoltaic Applications: Ab-Initio Results. Nanoscale Research Letters, 2010, 5, 1637-1649.	3.1	41
63	Electronic and optical properties of Si and Ge nanocrystals: An ab initio study. Superlattices and Microstructures, 2010, 47, 178-181.	1.4	1
64	Segregation, quantum confinement effect and band offset for [110] SiGe NWs. Physica Status Solidi (B): Basic Research, 2010, 247, 2096-2101.	0.7	16
65	Manyâ€body effects on the electronic and optical properties of Si nanowires from ab initio approaches. Physica Status Solidi (B): Basic Research, 2010, 247, 2089-2095.	0.7	7
66	Giant excitonic exchange splitting in Si nanowires: First-principles calculations. Physical Review B, 2010, 81, .	1.1	19
67	Test of long-range exchange-correlation kernels of time-dependent density functional theory at surfaces: Application toSi(111)2Ã—1. Physical Review B, 2010, 82, .	1.1	16
68	Convergence study of neutral and charged defect formation energies in Si nanowires. Physical Review B, 2010, 81, .	1.1	29
69	Ab initiooptoelectronic properties of SiGe nanowires: Role of many-body effects. Physical Review B, 2010, 82, .	1.1	22
70	SiGe nanowires: Structural stability, quantum confinement, and electronic properties. Physical Review B, 2009, 80, .	1.1	47
71	Reflectance-anisotropy spectroscopy and surface differential reflectance spectra at the Si(100) surface: Combined experimental and theoretical study. Physical Review B, 2009, 79, .	1.1	53
72	Electronic and optical properties of acetylene and ethylene on Si(001). Superlattices and Microstructures, 2009, 46, 240-245.	1.4	3

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73	Electronic properties and dielectric response of surfaces and nanowires of silicon from ab-initio approaches. Superlattices and Microstructures, 2009, 46, 234-239.	1.4	5
74	Theory of dielectric screening and electron energy loss spectroscopy at surfaces. Comptes Rendus Physique, 2009, 10, 560-574.	0.3	5
75	Reduced quantum confinement effect and electron-hole separation in SiGe nanowires. Physical Review B, 2009, 79, .	1.1	48
76	Ab initio electronic and optical spectra of free-base porphyrins: The role of electronic correlation. Journal of Chemical Physics, 2009, 131, 084102.	1.2	120
77	Experimental and Theoretical Investigation of the Pyrrole/Al(100) Interface. Journal of Physical Chemistry A, 2009, 113, 15193-15197.	1.1	7
78	Abâ€initio optical spectra of complex systems. Physica Status Solidi C: Current Topics in Solid State Physics, 2008, 5, 2543-2550.	0.8	2
79	Novel optoelectronic properties of simultaneously n- and p-doped silicon nanostructures. Superlattices and Microstructures, 2008, 44, 337-347.	1.4	26
80	From Si Nanowires to Porous Silicon: The Role of Excitonic Effects. Physical Review Letters, 2007, 98, 036807.	2.9	151
81	Ab-initio electronic and optical properties of low dimensional systems: From single particle to many-body approaches. Surface Science, 2007, 601, 2696-2701.	0.8	6
82	First-principles optical properties of silicon and germanium nanowires. Surface Science, 2007, 601, 2707-2711.	0.8	58
83	Geometry and electronic band structure of surfaces: the case of Ge(111):Sn and C(111). Applied Physics A: Materials Science and Processing, 2006, 85, 361-369.	1.1	10
84	Ab initiocalculation of many-body effects on the EEL spectrum of the C(100) surface. Physical Review B, 2006, 74, .	1.1	13
85	First-principles optical spectra of low dimensional systems. Physica Status Solidi (B): Basic Research, 2005, 242, 3032-3039.	0.7	4
86	Excitons in germanium nanowires: Quantum confinement, orientation, and anisotropy effects within a first-principles approach. Physical Review B, 2005, 72, .	1.1	93
87	Reflectance Anisotropy Spectra of the Diamond(100)â˜'(2Ã—1)Surface: Evidence of Strongly Bound Surface State Excitons. Physical Review Letters, 2005, 94, 087404.	2.9	34
88	The Betheâ€“Salpeter equation: a first-principles approach for calculating surface optical spectra. Journal of Physics Condensed Matter, 2004, 16, S4313-S4322.	0.7	28
89	Ab initio investigation of the adsorption of organic molecules at Si(111) and Si(100) surfaces. Surface Science, 2003, 532-535, 982-987.	0.8	11
90	Ab-initio study of the adsorption of acetylene on Si(001) surface. Physica Status Solidi C: Current Topics in Solid State Physics, 2003, 0, 2997-3001.	0.8	3

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91	First-principles study of acetylene adsorption on Si(100):â€‚â€‚The end-bridge structure. Physical Review B, 2003, 68, .	1.1	52
92	Anisotropy of surface optical properties at BN(110): Anab initiostudy. Physical Review B, 2002, 66, .	1.1	10
93	Optical properties of BN in cubic and layered hexagonal phases. Physical Review B, 2001, 64, .	1.1	84
94	Ab initio optical properties of BN in the cubic and in the layered hexagonal phase. Computational Materials Science, 2001, 22, 78-80.	1.4	8
95	AB-Initio Calculation of the optical Properties of BN(110) Surface.. Materials Research Society Symposia Proceedings, 2001, 677, 621.	0.1	1
96	Optical Properties of Germanium Quantum Dots. Physica Status Solidi (B): Basic Research, 2001, 224, 247-251.	0.7	8
97	All-Electron versus Pseudopotential Calculation of Optical Properties: The Case of GaAs. Physica Status Solidi A, 2001, 184, 101-104.	1.7	5
98	Theory for Modeling the Optical Properties of Surfaces. Physica Status Solidi A, 2001, 188, 1233-1242.	1.7	10
99	Many-Body Effects on the Electronic and Optical Properties of Bulk GaP. Physica Status Solidi A, 2001, 188, 1261-1266.	1.7	15
100	Ab initiopseudopotential calculation of the equilibrium structure of tin monoxide. Physical Review B, 2001, 64, .	1.1	36
101	Ab initiocalculation of second-harmonic-generation at theSi(100)surface. Physical Review B, 2001, 63, .	1.1	29
102	Reflectance anisotropy spectra of Cu and Ag (110) surfaces fromab initiotheory. Physical Review B, 2001, 64, .	1.1	25
103	First-principles calculations of electronic excitations in clusters. International Journal of Quantum Chemistry, 2000, 77, 951-960.	1.0	10
104	Structural and Optical Properties of the Ge(111)-(2Ã—1) Surface. Physical Review Letters, 2000, 85, 5440-5443.	2.9	68
105	Nonlocal density scheme for electronic-structure calculations. Physical Review B, 1999, 60, 11329-11335.	1.1	16
106	Exchange and correlation effects beyond the LDA on the dielectric function of silicon. Physical Review B, 1999, 60, 14224-14233.	1.1	42
107	Optical Properties of Germanium Nanocrystals. Physica Status Solidi A, 1999, 175, 23-31.	1.7	27
108	Monohydride Formation on Vicinal Si(001) Investigated by Reflectance Anisotropy Spectroscopy. Physica Status Solidi A, 1999, 175, 63-69.	1.7	3

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109	Theoretical Study of the Surface Optical Properties of Clean and Hydrogenated GaAs(110). Physica Status Solidi A, 1999, 175, 71-76.	1.7	3
110	Ab initiooptical properties of Si(100). Physical Review B, 1999, 60, 2522-2527.	1.1	74
111	Optical Properties of Cu-(110) Surface. Materials Research Society Symposia Proceedings, 1999, 579, 59.	0.1	0
112	Ab-Initio Calculation of the Optical Properties of Surfaces. Physica Status Solidi A, 1998, 170, 365-375.	1.7	6
113	Analytical expressions for the local-field factorG(q)and the exchange-correlation kernelKxc(r)of the homogeneous electron gas. Physical Review B, 1998, 57, 14569-14571.	1.1	120
114	Screening models and simplified GW approaches: Si & GaN as test cases. Solid State Communications, 1995, 95, 393-398.	0.9	19
115	The electronic structure of gallium nitride. Physica B: Condensed Matter, 1993, 185, 404-409.	1.3	62
116	Optical absorption of Tl+ ions in KMgF3 crystals. Journal of Physics and Chemistry of Solids, 1993, 54, 1035-1041.	1.9	16
117	Hydrogen covered Si(111) surfaces. Surface Science, 1992, 269-270, 879-885.	0.8	35
118	Optical properties of (F2+)HandF-aggregate centers in NaCl:OHâ˜’crystals. Physical Review B, 1991, 44, 12189-12196.	1.1	4
119	VUV excitation levels of Cr3+ luminescence in indium fluoride garnet. Solid State Communications, 1990, 76, 1051-1054.	0.9	14