Simone Sanna

List of Publications by Year
in descending order

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117 papers	2,377 citations	218677 26 h-index	254184 43 g-index
120 all docs	120 docs citations	120 times ranked	2320 citing authors

#	Article	IF	Citations
1	niobate<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>X</mml:mi></mml:math>-cut,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Y</mml:mi></mml:math>-cut, and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Z</mml:mi></mml:math>-cut surfaces fromab initiotheory. Physical Re	3.2	117
2	Incoherent Electronâ"Phonon Scattering in Octanethiols. Nano Letters, 2004, 4, 2109-2114.	9.1	106
3	Optically excited structural transition in atomic wires on surfaces at the quantum limit. Nature, 2017, 544, 207-211.	27.8	99
4	Raman scattering efficiency in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LiTaO</mml:mi><mml:mn>3</mml:mn></mml:msub></m xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LiNbO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2015, 91, .	3.2	94
5	Do we know the band gap of lithium niobate?. Physica Status Solidi C: Current Topics in Solid State Physics, 2010, 7, 362-365.	0.8	93
6	Barium titanate ground- and excited-state properties from first-principles calculations. Physical Review B, 2011, 83, .	3.2	85
7	Density-functional based tight-binding study of small gold clusters. New Journal of Physics, 2006, 8, 9-9.	2.9	72
8	Rare-earth defect pairs in GaN:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>LDA</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math> Physical Review B, 2009, 80, .	3.2	70
9	Atomistic Picture of Charge Density Wave Formation at Surfaces. Physical Review Letters, 2012, 109, 186101.	7.8	69
10	LiNbO₃surfaces from a microscopic perspective. Journal of Physics Condensed Matter, 2017, 29, 413001.	1.8	58
11	Self-Interaction and Strong Correlation in DFTBâ€. Journal of Physical Chemistry A, 2007, 111, 5671-5677.	2.5	52
12	Defect complexes in congruent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">LiNbO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>and their optical signatures. Physical Review B, 2015, 91, .	3.2	45
13	Temperature Driven Phase Transition at the Antimonene/Bi₂Se₃ van der Waals Heterostructure. ACS Nano, 2019, 13, 10481-10489.	14.6	45
14	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>LiNbO</mml:mtext><mml:mn>3</mml:mn></mml:ms structure: Many-body interactions, spin-orbit coupling, and thermal effects. Physical Review B, 2016, 93, .	3.2	41
15	Tunable variation of the electron effective mass and exciton radius in hydrogenatedGaAs1â"xNx. Physical Review B, 2004, 69, .	3.2	40
16	Optical response of stoichiometric and congruent lithium niobate from first-principles calculations. Physical Review B, 2013, 87, .	3.2	39
17	IntrinsicLiNbO3point defects from hybrid density functional calculations. Physical Review B, 2014, 89, .	3.2	36
18	Validity of the Slater-Janak transition-state model within the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>LDA</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math> Physical Review B, 2008, 78, .	3.2	34

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19	Polarization-dependent water adsorption on the LiNbO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>(0001) surface. Physical Review B, 2012, 86, .	3.2	34
20	Phonon dispersion and zero-point renormalization of LiNbO₃from density-functional perturbation theory. Journal of Physics Condensed Matter, 2015, 27, 385402.	1.8	34
21	Atomic-resolution imaging of the polar (000<mml:math) surface of LiNbO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>in aqueous solution by frequency modulation atomic force microscopy. Physical Review B, 2012, 86, .	3.2	33
22	Modeling intrinsic defects in LiNbO₃ within the Slater-Janak transition state model. Journal of Chemical Physics, 2014, 140, 234113.	3.0	33
23	Polaronic deformation at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mtext>Fe</mml:mtext><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msup></mml:math>site in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>Fe:LiNbO</mml:mtext><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2015, 91, .	3.2	33
24	Formation of Hydroxyl Groups at Calcium-Silicate-Hydrate (C-S-H): Coexistence of Caâ€“OH and Siâ€“OH on Wollastonite(001). Journal of Physical Chemistry C, 2014, 118, 8007-8013.	3.1	28
25	Temperature dependent LiNbO3(0001): Surface reconstruction and surface charge. Applied Surface Science, 2014, 301, 70-78.	6.1	28
26	Rare-earth silicide thin films on the Si(111) surface. Physical Review B, 2016, 93, .	3.2	28
27	Vibrational properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>LiNb</mml:mi><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>mixed crystals. Physical Review B, 2016, 93, .	3.2	26
28	A theoretical study of erbium in GaN. Physica B: Condensed Matter, 2006, 376-377, 512-515.	2.7	25
29	Inâ€Si(111)(4â€‰Ã—â€‰1)/(8â€‰Ã—â€‰2) nanowires: Electron transport, entropy, and metalâ€insulator transition. Physica Status Solidi (B): Basic Research, 2012, 249, 343-359.	1.5	25
30	Imaging of the Ferroelectric Domain Structures by Confocal Raman Spectroscopy. Ferroelectrics, 2011, 420, 44-48.	0.6	24
31	Theoretical study of rare earth point defects in GaN. Physica Status Solidi C: Current Topics in Solid State Physics, 2008, 5, 2358-2360.	0.8	23
32	Charge compensation by long-period reconstruction in strongly polar lithium niobate surfaces. Physical Review B, 2013, 88, .	3.2	23
33	Grand canonical Peierls transition in In/Si(111). Physical Review B, 2016, 93, .	3.2	23
34	Whiteâ€Light Generation Upon Inâ€Situ Amorphization of Single Crystals of [{(Me 3 P) 3 AuSn}(PhSn) 3 S 6] and [{(Et 3 P) 3 AgSn}(PhSn) 3 S 6]. Advanced Optical Materials, 2019, 7, 1801793.	7.3	23
35	Imaging of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mn>180</mml:mn></mml:mrow><mml:mo> ferroelectric domain walls in uniaxial ferroelectrics by confocal Raman spectroscopy: Unraveling the contrast mechanism. Physical Review Materials, 2018, 2, .	2.4	23
36	LiTaO3 phonon dispersion and ferroelectric transition calculated from first principles. Physica Status Solidi (B): Basic Research, 2016, 253, 683-689.	1.5	22

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37	Tuning the conductivity along atomic chains by selective chemisorption. Physical Review B, 2017, 95, .	3.2	22
38	How One-Dimensional Are Atomic Gold Chains on a Substrate?. Journal of Physical Chemistry C, 2018, 122, 25580-25588.	3.1	22
39	Efficient tight-binding approach for the study of strongly correlated systems. Physical Review B, 2007, 76, .	3.2	20
40	Influence of Na adsorption on the quantum conductance and metal-insulator transition of the In-Si(111)(4Ã—1)â€“(8Ã—2) nanowire array. Physical Review B, 2011, 84, .	3.2	19
41	Polarization-dependent methanol adsorption on lithium niobate Z-cut surfaces. Physical Review B, 2012, 86, .	3.2	19
42	Consistent Atomic Geometries and Electronic Structure of Five Phases of Potassium Niobate from Density-Functional Theory. Advances in Materials Science and Engineering, 2017, 2017, 1-13.	1.8	19
43	Probing quasi-one-dimensional band structures by plasmon spectroscopy. Physical Review B, 2018, 97, .	3.2	19
44	Evaluation of similarities and differences of LiTaO₃ and LiNbO₃ based on high-T-conductivity, nonlinear optical fs-spectroscopy and ab initio modeling of polaronic structures. New Journal of Physics, 2021, 23, 033016.	2.9	19
45	Ferroelectric phase transition in LiNbO₃: Insights from molecular dynamics. IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, 2012, 59, 1925-1928.	3.0	18
46	Extrinsic doping on the atomic scale: Tuning metallicity in atomic Au chains. Physical Review B, 2018, 98, .	3.2	17
47	Topologization of Î²-antimonene on Bi2Se3 via proximity effects. Scientific Reports, 2020, 10, 14619.	3.3	17
48	Si(775)-Au atomic chains: Geometry, optical properties, and spin order. Physical Review Materials, 2017, 1, .	2.4	17
49	Modeling LiNbO₃ Surfaces at Ambient Conditions. Journal of Physical Chemistry C, 2014, 118, 10213-10220.	3.1	16
50	Vibration eigenmodes of the Au- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:mn>5</mml:mn><mml:mo>Ã—</mml /Si(111) surface studied by Raman spectroscopy and first-principles calculations. Physical Review B, 2016, 94, .	3.2	16
51	Water Splitting Reaction at Polar Lithium Niobate Surfaces. ACS Omega, 2019, 4, 3850-3859.	3.5	16
52	An Efficient LDA+UBased Tight Binding Approachâ€. Journal of Physical Chemistry A, 2007, 111, 5665-5670.	2.5	15
53	Adsorption of OH and H at the LiNbO₃(0001) surface. Physica Status Solidi C: Current Topics in Solid State Physics, 2012, 9, 1361-1365.	0.8	15
54	Vibration-Driven Self-Doping of Dangling-Bond Wires on Si(553)-Au Surfaces. Physical Review Letters, 2020, 124, 146802.	7.8	15

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55	Atomic size effects studied by transport in single silicide nanowires. Physical Review B, 2016, 93, .	3.2	14
56	Towards Understanding the Reactivity and Optical Properties of Organosilicon Sulfide Clusters. Angewandte Chemie - International Edition, 2021, 60, 1176-1186.	13.8	14
57	Enforced Long-Range Order in 1D Wires by Coupling to Higher Dimensions. Physical Review Letters, 2021, 126, 106101.	7.8	14
58	Polaron optical absorption in congruent lithium niobate from time-dependent density-functional theory. Physical Review Materials, 2017, 1, .	2.4	13
59	Density-functional tight-binding calculations of electronic states associated with grain boundaries in GaN. Physical Review B, 2005, 71, .	3.2	12
60	Ab initioinvestigation of the LiNbO3(0001) surface. Physica Status Solidi C: Current Topics in Solid State Physics, 2010, 7, 145-148.	0.8	12
61	Lattice constant, effective mass, and gap recovery in hydrogenatedGaAs1â^'xNx. Physical Review B, 2004, 69, .	3.2	11
62	Comparison between experimental and theoretical determination of the local structure of theGaAs1â^'yNydilute nitride alloy. Physical Review B, 2005, 71, .	3.2	11
63	Localised Phonon Modes at LiNbO₃(0001) Surfaces. Ferroelectrics, 2011, 419, 1-8.	0.6	11
64	Liquid Crystal (8CB) Molecular Adsorption on Lithium Niobate Z-Cut Surfaces. Journal of Physical Chemistry C, 2015, 119, 9342-9346.	3.1	11
65	Modeling atomic force microscopy at LiNbO 3 surfaces from first-principles. Computational Materials Science, 2015, 103, 145-150.	3.0	11
66	Amorphous Molecular Materials for Directed Supercontinuum Generation. ChemPhotoChem, 2021, 5, 1033-1041.	3.0	11
67	Unraveling the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mtext>LiNbO</mml:mtext></mml:mrow><mml: surface by atomic force microscopy and density functional theory. Physical Review B, 2014, 89, .	3.2	10
68	Temperature-Dependent Hole Mobility and Its Limit in Crystal-Phase P3HT Calculated from First Principles. Journal of Physical Chemistry B, 2016, 120, 5572-5580.	2.6	10
69	Vibrational properties of the Au-(<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 187 Td (xmlns:mml="http://www.w3.org/	3.2	10
70	Optical properties of titanium-doped lithium niobate from time-dependent density-functional theory. Physical Review Materials, 2017, 1, .	2.4	10
71	Plasmon spectroscopy: Robust metallicity of Au wires on Si(557) upon oxidation. Physical Review Materials, 2018, 2, .	2.4	10
72	Quasiparticle and excitonic effects in the optical response of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>KNbO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review Materials, 2019, 3, .	2.4	10

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73	GaN/LiNbO3 (0001) interface formation calculated from first-principles. Applied Surface Science, 2010, 256, 5740-5743.	6.1	9
74	Vibrational properties of the LiNbO3 z-surfaces. IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, 2011, 58, 1751-1756.	3.0	9
75	Linear and nonlinear optical response of LiNbO₃ calculated from first principles. IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, 2012, 59, 1929-1933.	3.0	9
76	Strain-induced quasi-one-dimensional rare-earth silicide structures on Si(111). Physical Review B, 2016, 94, .	3.2	9
77	Structure and one-dimensional metallicity of rare-earth silicide nanowires on Si(001). Physical Review B, 2019, 99, .	3.2	9
78	Plasmon Localization by H-Induced Band Switching. Journal of Physical Chemistry C, 2020, 124, 958-967.	3.1	9
79	Microscopic structure and energy transfer of vacancy-related defect pairs with Erbium in wide-gap semiconductors. Optical Materials, 2011, 33, 1041-1044.	3.6	8
80	FriggeetÂal.Reply:. Physical Review Letters, 2013, 111, 149602.	7.8	8
81	Towards Understanding the Reactivity and Optical Properties of Organosilicon Sulfide Clusters. Angewandte Chemie, 2021, 133, 1196-1206.	2.0	8
82	Clusterâ€Glass for Lowâ€Cost Whiteâ€Light Emission. Advanced Materials, 2022, 34, .	21.0	8
83	Vibrational Fingerprints of LiNbO₃-LiTaO₃Mixed Crystals. Ferroelectrics, 2013, 447, 63-68.	0.6	7
84	Evolution of Topological Surface States Following Sb Layer Adsorption on Bi2Se3. Materials, 2021, 14, 1763.	2.9	7
85	LiNb_{1-x}Ta_xO₃Electronic Structure and Optical Response fromFirst-PrinciplesCalculations. Ferroelectrics, 2013, 447, 78-85.	0.6	6
86	Temperature stabilizes rough Au/Ge(001) surface reconstructions. Surface Science, 2018, 667, 101-104.	1.9	6
87	Surface localized phonon modes at the Si(553)-Au nanowire system. Physical Review B, 2021, 103, .	3.2	6
88	Magnetic characterization of conductance electrons in GaN. Physica Status Solidi (B): Basic Research, 2010, 247, 1728-1731.	1.5	5
89	Nonlinear optical response of ferroelectric oxides: First-principles calculations within the time and frequency domains. Physical Review Materials, 2022, 6, .	2.4	5
90	GaN growth on LiNbO3 (0001) - a first-principles simulation. Physica Status Solidi C: Current Topics in Solid State Physics, 2010, 7, 2272-2274.	0.8	4

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91	Improved parameterization of the quantum harmonic oscillator model based on localized wannier functions to describe Van der Waals interactions in density functional theory. International Journal of Quantum Chemistry, 2016, 116, 1160-1165.	2.0	4
92	Impact of carbon-ion implantation on the nonlinear optical susceptibility of LiNbO_3. Optics Express, 2017, 25, 21444.	3.4	4
93	Continuous crossover from two-dimensional to one-dimensional electronic properties for metallic silicide nanowires. Physical Review B, 2020, 102, .	3.2	4
94	Vibrational Raman spectroscopy on adsorbate-induced low-dimensional surface structures. Surface Science Reports, 2020, 75, 100480.	7.2	4
95	Tetraphenyl Tetrel Molecules and Molecular Crystals: From Structural Properties to Nonlinear Optics. Journal of Physical Chemistry C, 2022, 126, 3713-3726.	3.1	4
96	Vibration signatures of the structural phase transition of Sn/Ge(111) compared to Sn/Si(111). Physical Review B, 2019, 100, .	3.2	3
97	Spectroscopic Analysis of Rare-Earth Silicide Structures on the Si(111) Surface. Materials, 2021, 14, 4104.	2.9	3
98	Theoretical study of stability, epitaxial formation, and phase transformations of two-dimensional pnictogen allotropes. Physical Review B, 2021, 104, .	3.2	3
99	Amorphous Molecular Materials for Directed Supercontinuum Generation. ChemPhotoChem, 2021, 5, 1029.	3.0	2
100	Adamantanes as White-Light Emitters: Controlling the Arrangement and Functionality by External Coulomb Forces. Journal of Physical Chemistry C, 0, , .	3.1	2
101	Co-Doping of Er-Doped SiC with Oxygen â€“ A Promising Way Towards Efficient 1540 nm Emission at Room Temperature?. Materials Science Forum, 2006, 527-529, 655-658.	0.3	1
102	Theoretical investigation of Er-O co-doping in hexagonal GaN. Materials Research Society Symposia Proceedings, 2011, 1342, 73.	0.1	1
103	Surface Resonant Raman Scattering from Cu(110). Physical Review Letters, 2022, 128, .	7.8	1
104	Ferroelectric phase transition in LiNbO<inf>3</inf>: Insights from molecular dynamics. , 2011, , .		0
105	LiNbO<inf>3</inf> linear and nonlinear optical response from first-principles calculations. , 2011, , .		0
106	Vibrational fingerprints of LiNbO<inf>3</inf>-LiTaO<inf>3</inf> mixed crystals. , 2012, , .		0
107	Bound electron polarons in lithium niobate. , 2015, , .		0
108	Frontispiz: Towards Understanding the Reactivity and Optical Properties of Organosilicon Sulfide Clusters. Angewandte Chemie, 2021, 133, .	2.0	0

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109	Frontispiece: Towards Understanding the Reactivity and Optical Properties of Organosilicon Sulfide Clusters. Angewandte Chemie - International Edition, 2021, 60, .	13.8	0
110	Lithium Niobate Dielectric Function and Second-Order Polarizability Tensor From Massively Parallel Ab Initio Calculations. , 2013, , 93-104.		0
111	Polarization Dependent Water Adsorption on the Lithium Niobate Z-Cut Surfaces. , 2013, , 155-166.		0
112	Surface Charge of Clean LiNbO3 Z-Cut Surfaces. , 2015, , 163-178.		0
113	Submonolayer Rare Earth Silicide Thin Films on the Si(111) Surface. , 2016, , 163-175.		0
114	Tuning the Conductivity of Metallic Nanowires by Hydrogen Adsorption. , 2021, , 133-146.		0
115	Au adsorption on stepped Si(hhk)-Au surfaces. Surface Science, 2022, 718, 122010.	1.9	0
116	Adsorbateâ€induced modifications in the optical response of Si(553)â€Au nanowires. Physica Status Solidi - Rapid Research Letters, 0, , .	2.4	0
117	Electronic phase transitions in quasi-one-dimensional atomic chains: Au wires on Si(553). Physical Review B, 2022, 105, .	3.2	0