

Paola Alippi

List of Publications by Year in descending order

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65
papers

1,484
citations

361045

20
h-index

315357

38
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65
all docs

65
docs citations

65
times ranked

2138
citing authors

#	ARTICLE	IF	CITATIONS
1	Ab initio study of the electronic states induced by oxygen vacancies in rutile and anatase TiO_2 . Physical Review B, 2008, 78, .	1.1	239
2	Deep versus Shallow Behavior of Intrinsic Defects in Rutile and Anatase TiO_2 Polymorphs. Journal of Physical Chemistry C, 2010, 114, 21694-21704.	1.5	138
3	Strained Tetragonal States and Bain Paths in Metals. Physical Review Letters, 1997, 78, 3892-3895.	2.9	129
4	Evidence of Cobalt-Vacancy Complexes in ZnO Dilute Magnetic Semiconductors. Physical Review Letters, 2011, 107, 127206.	2.9	86
5	A phase-field approach to the simulation of the excimer laser annealing process in Si. Journal of Applied Physics, 2004, 95, 4806-4814.	1.1	69
6	Oxygen vacancies and OH species in rutile and anatase TiO_2 polymorphs. Catalysis Today, 2009, 144, 177-182.	2.2	67
7	Properties of hydrogen and hydrogen-vacancy complexes in the rutile phase of titanium dioxide. Physical Review B, 2009, 80, .	1.1	60
8	The electronic structure of $\mu\text{-Ga}_2\text{O}_3$. APL Materials, 2019, 7, .	2.2	49
9	Tetragonal states from epitaxial strain on metal films. Physical Review B, 1998, 57, 1971-1975.	1.1	45
10	Atomic-scale characterization of boron diffusion in silicon. Physical Review B, 2001, 64, .	1.1	43
11	Interfacial Engineering of P3HT/ZnO Hybrid Solar Cells Using Phthalocyanines: A Joint Theoretical and Experimental Investigation. Advanced Energy Materials, 2014, 4, 1301694.	10.2	42
12	Zinc Oxide-Zinc Phthalocyanine Interface for Hybrid Solar Cells. Journal of Physical Chemistry C, 2012, 116, 15439-15448.	1.5	36
13	A hybrid zinc phthalocyanine/zinc oxide system for photovoltaic devices: a DFT and TDDFT theoretical investigation. Journal of Materials Chemistry, 2012, 22, 440-446.	6.7	32
14	Lattice-strain field induced by $\{311\}$ self-interstitial defects in silicon. Physical Review B, 2000, 62, 1815-1820.	1.1	27
15	Ferromagnetism and Conductivity in Hydrogen Irradiated Co-Doped ZnO Thin Films. ACS Applied Materials & Interfaces, 2016, 8, 12925-12931.	4.0	25
16	Clusters and Magnetic Anchoring Points in (Ga,Fe)N Condensed Magnetic Semiconductors. Physical Review Letters, 2011, 107, 196401.	2.9	23
17	Material modifications induced by laser annealing in two-dimensional structures. Applied Physics Letters, 2004, 84, 4738-4740.	1.5	22
18	Role of light scattering in excimer laser annealing of Si. Applied Physics Letters, 2005, 86, 161905.	1.5	21

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19	Energetics and diffusivity of indium-related defects in silicon. <i>Physical Review B</i> , 2004, 69, .	1.1	20
20	How much room for BiGa heteroantisites in GaAs $\hat{1}^{\wedge}$ <i>x</i> <i>/i>Bi<i>x</i>?. <i>Applied Physics Letters</i>, 2011, 99, .</i>	1.5	20
21	Supramolecular and Chiral Effects at the Titanyl Phthalocyanine/Ag(100) Hybrid Interface. <i>Journal of Physical Chemistry C</i> , 2014, 118, 5255-5267.	1.5	20
22	Neutral boron-interstitial clusters in crystalline silicon. <i>Physical Review B</i> , 2004, 69, .	1.1	19
23	Bound states of the Fe impurity in wurtzite GaN from hybrid density-functional calculations. <i>Physical Review B</i> , 2011, 84, .	1.1	19
24	Triple junctions and elastic stability of polycrystalline silicon. <i>Physical Review B</i> , 2000, 63, .	1.1	17
25	The effect of Co doping on the conductive properties of ferromagnetic Zn _x Co _{1-x} O films. <i>Journal of Materials Chemistry C</i> , 2015, 3, 10188-10194.	2.7	17
26	Structural characterization of Ni ₂ Si pseudoepitaxial transrotational structures on [001] Si. <i>Acta Crystallographica Section B: Structural Science</i> , 2006, 62, 729-736.	1.8	14
27	Effects of cobalt substitution on ZnO surface reactivity and electronic structure. <i>Journal of Materials Chemistry C</i> , 2019, 7, 8364-8373.	2.7	13
28	Role of the indium-carbon interaction on In diffusion and activation in Si. <i>Applied Physics Letters</i> , 2003, 83, 1956-1958.	1.5	12
29	Electrical activation phenomena induced by excimer laser annealing in B-implanted silicon. <i>Applied Physics Letters</i> , 2004, 85, 2268-2270.	1.5	11
30	Reorientable dipolar and anomalous screening in CuCa_3 Physical Review B, 2010, 81, .	1.1	11
31	Unexpected Rotamerism at the Origin of a Chessboard Supramolecular Assembly of Ruthenium Phthalocyanine. <i>Chemistry - A European Journal</i> , 2017, 23, 16319-16327.	1.7	11
32	Energetics and diffusivity of atomic boron in silicon by density-functional-based tight-binding simulations. <i>Computational Materials Science</i> , 2001, 22, 44-48.	1.4	10
33	Magnetism and unusual Cu valency in quadruple perovskites. <i>European Physical Journal B</i> , 2012, 85, 1.	0.6	10
34	Impurity-vacancy complexes and ferromagnetism in doped sesquioxides. <i>Physical Review B</i> , 2014, 89, .	1.1	9
35	Experimental determination of the local geometry around In and In-C complexes in Si. <i>Applied Physics Letters</i> , 2006, 88, 212102.	1.5	8
36	Electronic structure of hydrogenated diamond: Microscopical insight into surface conductivity. <i>Physical Review B</i> , 2016, 94, .	1.1	8

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37	Disclosing the Nature of Asymmetric Interface Magnetism in Co/Pt Multilayers. ACS Applied Materials & Interfaces, 2022, 14, 12766-12776.	4.0	8
38	A multi-scale atomistic study of the interstitials agglomeration in crystalline Si. Nuclear Instruments & Methods in Physics Research B, 2001, 178, 154-159.	0.6	7
39	Native point defects in $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$. IOP Conference Series: Materials Science and Engineering, 2010, 8, 012015.	0.3	7
40	Connections between local and macroscopic properties in solids: The case of N in III-V-N alloys. Physical Review B, 2014, 89, .	1.1	7
41	A Ru–Ru pair housed in ruthenium phthalocyanine: the role of a “cage”-architecture in the molecule coupling with the Ag(111) surface. Physical Chemistry Chemical Physics, 2017, 19, 1449-1457.	1.3	7
42	Alkali-metal plasmons, pseudopotentials, and optical sum rules. Physical Review B, 1997, 55, 13835-13841.	1.1	6
43	Atomic scale computer aided design for novel semiconductor devices. Computational Materials Science, 2003, 27, 10-15.	1.4	6
44	Electronic Structure of Bulk and Defected $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$. ECS Transactions, 2006, 3, 291-297.	0.3	5
45	Technology Computer Aided Design of Ultra-shallow Junctions in Si Devices Formed by Laser Annealing Processes. Materials Research Society Symposia Proceedings, 2004, 810, 269.	0.1	4
46	The effect of thermal treatments on the local geometry around indium in In and In+C high dose implanted Si. Nuclear Instruments & Methods in Physics Research B, 2006, 253, 59-62.	0.6	4
47	Impact of the Substrate Work Function on Self-Assembling and Electronic Structure of Adsorbed Ruthenium Phthalocyanine. Journal of Physical Chemistry C, 2020, 124, 23295-23306.	1.5	4
48	A systematic study of the valence electronic structure of cyclo(Gly–Phe), cyclo(Trp–Tyr) and cyclo(Trp–Trp) dipeptides in the gas phase. Physical Chemistry Chemical Physics, 2021, 23, 26793-26805.	1.3	4
49	From Point to Extended Defects in Silicon: A Theoretical Study. Solid State Phenomena, 2001, 85-86, 177-202.	0.3	2
50	Ultra-shallow junction by laser annealing: Integration issues and modelling. Nuclear Instruments & Methods in Physics Research B, 2006, 253, 1-8.	0.6	2
51	Effects of interface bonding on the conductance of metal–carbon nanotube–metal systems. Materials Science and Engineering C, 2007, 27, 1102-1107.	3.8	2
52	Multigap absorption in $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ and the prediction capability of fab initio methods. Physical Review B, 2014, 90, .	1.1	2
53	Ab Initio Investigations of Textured Ni_2Si Films on Silicon. ECS Transactions, 2006, 3, 149-155.	0.3	1
54	Temperature Dependent Reaction of Thin Ni-Silicide Transrotational Layers on [001]Si. , 2007, , .		1

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55	Magnetic and X-ray absorption investigations of Co-doped ZnO films. Journal of Physics: Conference Series, 2010, 200, 072025.	0.3	1
56	Influence of the surface structure on the magnetic properties of Zn _{1-x} CoxO. Applied Physics Letters, 2012, 101, 252101.	1.5	1
57	Defect-induced magnetism in cobalt-doped ZnO epilayers. , 2014, , .		1
58	Understanding Structure and Electronic Properties of Extended Self-Interstitial Defects in Silicon. Materials Research Society Symposia Proceedings, 1998, 538, 353.	0.1	0
59	Atomistic Study of Boron Clustering in Silicon. Solid State Phenomena, 2002, 82-84, 163-170.	0.3	0
60	Indium in silicon: interactions with native defects and with C impurities. Materials Research Society Symposia Proceedings, 2004, 810, 311.	0.1	0
61	Role of C and Ge in the electrical activation of In implanted in Silicon. Materials Research Society Symposia Proceedings, 2004, 810, 404.	0.1	0
62	Computational methods for the simulation of the excimer laser annealing in MOS technology. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2004, 114-115, 100-104.	1.7	0
63	Excimer Laser Annealing of Ion-Implanted Silicon: Dopant Activation, Diffusion and Defect Formation. , 2007, , .		0
64	The Site of In Dopants in Si. AIP Conference Proceedings, 2007, , .	0.3	0
65	XAS, XES and DFT simulations to bridge local and macroscopic properties in GaAsN. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1520-C1520.	0.0	0