Francesco Filippone

List of Publications by Year
in descending order

58 papers	1,561 citations	304368 22 h-index	301761 39 g-index
58 all docs	58 docs citations	58 times ranked	2041 citing authors

#	Article	IF	Citations
1	Ab initiostudy of the electronic states induced by oxygen vacancies in rutile and anatase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2008, 78, .	1.1	239
2	Deep versus Shallow Behavior of Intrinsic Defects in Rutile and Anatase TiO₂ Polymorphs. Journal of Physical Chemistry C, 2010, 114, 21694-21704.	1.5	138
3	Reaction Intermediates in the Photoreduction of Oxygen Molecules at the (101) TiO2(Anatase) Surface. Journal of the American Chemical Society, 2006, 128, 13772-13780.	6.6	80
4	Short Hydrogen Bonds at the Water/TiO₂ (Anatase) Interface. Journal of Physical Chemistry C, 2008, 112, 13579-13586.	1.5	71
5	Oxygen vacancies and OH species in rutile and anatase TiO2 polymorphs. Catalysis Today, 2009, 144, 177-182.	2.2	67
6	Properties of hydrogen and hydrogenâ€“vacancy complexes in the rutile phase of titanium dioxide. Physical Review B, 2009, 80, .	1.1	60
7	Nitrogen-hydrogen complex inGaAsxN1â^'xrevealed by x-ray absorption spectroscopy. Physical Review B, 2005, 71, .	1.1	56
8	Structure and Passivation Effects of Mono- and Dihydrogen Complexes inGaAsyN1â^'yAlloys. Physical Review Letters, 2002, 89, 216401.	2.9	52
9	Local structure of (Ga,Fe)N and (Ga,Fe)N:Si investigated by x-ray absorption fine structure spectroscopy. Physical Review B, 2009, 79, .	1.1	42
10	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
11	Vibrational spectroscopy of hydrogenatedGaAs1â^'yNy:â€ƒA structure-sensitive test of anH2*(N)model. Physical Review B, 2004, 69, .	1.1	41
12	Structural and Electronic Properties of Sodalite: An ab Initio Molecular Dynamics Study. The Journal of Physical Chemistry, 1995, 99, 12883-12891.	2.9	40
13	Lattice relaxation by atomic hydrogen irradiation ofIIIâ^'Nâ^'Vsemiconductor alloys. Physical Review B, 2003, 68, .	1.1	38
14	Charged chromophoric units in protonated rare-gas clusters: A dynamical simulation. Europhysics Letters, 1998, 44, 585-591.	0.7	36
15	Zinc Oxideâ€“Zinc Phthalocyanine Interface for Hybrid Solar Cells. Journal of Physical Chemistry C, 2012, 116, 15439-15448.	1.5	36
16	Nitrogen passivation by atomic hydrogen inGaAsyN1â^'yandInxGa1â^'xAsyN1â^'yalloys. Physical Review B, 2003, 68, .	1.1	34
17	A hybrid zinc phthalocyanine/zinc oxide system for photovoltaic devices: a DFT and TDDFPT theoretical investigation. Journal of Materials Chemistry, 2012, 22, 440-446.	6.7	32
18	Ab initio Theoretical Investigation of Phthalocyanineâ^'Semiconductor Hybrid Systems. Chemistry of Materials, 2009, 21, 4555-4567.	3.2	27

#	Article	IF	Citations
19	Competitive shell-filling in protonated helium clusters. Chemical Physics, 1999, 241, 203-212.	0.9	26
20	H-Induced Dangling Bonds in Hâ€“Isoelectronic-Impurity Complexes Formed inGaAs1âˆ’yNyAlloys. Physical Review Letters, 2007, 98, 206403.	2.9	25
21	Vibrational analysis from linear response theory. Chemical Physics Letters, 2001, 345, 179-182.	1.2	23
22	Clusters and Magnetic Anchoring Points in (Ga,Fe)N Condensed Magnetic Semiconductors. Physical Review Letters, 2011, 107, 196401.	2.9	23
23	Reaction intermediates and pathways in the photoreduction of oxygen molecules at the (101) TiO2 (anatase) surface. Catalysis Today, 2007, 129, 169-176.	2.2	22
24	Photocatalytic reduction of oxygen molecules at the (100) TiO2 anatase surface. Surface Science, 2005, 577, 59-68.	0.8	21
25	Local structure of nitrogen-hydrogen complexes in dilute nitrides. Physical Review B, 2009, 79, .	1.1	21
26	Supramolecular and Chiral Effects at the Titanyl Phthalocyanine/Ag(100) Hybrid Interface. Journal of Physical Chemistry C, 2014, 118, 5255-5267.	1.5	20
27	Bound states of the Fe impurity in wurtzite GaN from hybrid density-functional calculations. Physical Review B, 2011, 84, .	1.1	19
28	Use of Auger parameter and Wagner plot in the characterization of Cu-ZSM-5 catalysts. Surface and Interface Analysis, 2001, 31, 249-254.	0.8	18
29	Oxide electronic polarizabilities and aluminum coordination at the outer surface of zeolites obtained by X-ray photoelectron spectroscopy. Applied Surface Science, 1998, 135, 150-162.	3.1	15
30	A novel implicit Newtonâ€“Raphson geometry optimization method for density functional theory calculations. Journal of Chemical Physics, 2001, 115, 636-642.	1.2	15
31	Controlling the Magnetic Properties of a Single Phthalocyanine Molecule through its Strong Coupling with the GaAs Surface. Journal of Physical Chemistry Letters, 2010, 1, 2757-2762.	2.1	15
32	Local structure of Mn in hydrogenated<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ga</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:mr Physical Review B, 2008, 78, .	1.1	14
33	Theoretical Design of Coupled Organic-Inorganic Systems. Physical Review Letters, 2008, 101, 126805.	2.9	14
34	Structure, electronic properties, and formation mechanisms of hydrogen-nitrogen complexes inGaPyN1âˆ’yalloys. Physical Review B, 2004, 69, .	1.1	13
35	Structure and dynamics of small protonated rare-gas clusters using quantum and classical methods. Computer Physics Communications, 2002, 145, 78-96.	3.0	12
36	Local and lattice relaxations in hydrogenatedGaAsyN1âˆ’yalloys. Physical Review B, 2003, 68, .	1.1	12

#	Article	IF	Citations
37	ation of four-hydrogen complexes in In-rich In<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>Ga<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>N		

#	Article	IF	Citations
55	Tuning of the optical properties of In-rich In[sub x]Ga[sub 1â^'x]N (x=0.82â^'0.49) alloys by light-ion irradiation at low energy. , 2013, , .		0
56	Selective Effects of the Host Matrix in Hydrogenated InGaAsN Alloys: Toward an Integrated Matrix/Defect Engineering Paradigm. Advanced Functional Materials, 2022, 32, 2108862.	7.8	0
57	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
58	Independence of solitary-cation properties on the atomic neighborhood in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>In</mml:mi><mml:mrow><mml:mn>1</mml mathvariant="normal">N</mml:mi></mml:mrow></mml:math> alloys: A novel perspective for material engineering. Physical Review Materials, 2017, 1, .	0.9	0