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	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
2	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
3	Opposite Hydrogen Behaviors in GaAsN and InAsN Alloys: Band Gap Opening Versus Donor Doping. Journal of Physical Chemistry C, 2020, 124, 19240-19251.	1.5	5
4	A Ruâ€“Ru pair housed in ruthenium phthalocyanine: the role of a â€œcageâ€•architecture in the molecule coupling with the Ag(111) surface. Physical Chemistry Chemical Physics, 2017, 19, 1449-1457.	1.3	7
5	Unexpected Rotamerism at the Origin of a Chessboard Supramolecular Assembly of Ruthenium Phthalocyanine. Chemistry - A European Journal, 2017, 23, 16319-16327.	1.7	11
6	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
7	Genesis of â€œSolitary Cationsâ€•Induced by Atomic Hydrogen. Advanced Functional Materials, 2015, 25, 5353-5359.	7.8	6
8	Nearly-free electronlike surface resonance of a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi><mml:mo>âˆ’</mml:mo><mml:msub><mml:mi mathvariant="normal">Si</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mo>(</mml:mo><mml:mn>0001</mml:mn><mml:mo>) Physical Review B, 2015, 91, .	1.1	11
9	Interaction of silicene with<i>Î²</i>-Si₃N₄(0001)/Si(111) substrate; energetics and electronic properties. Journal of Physics Condensed Matter, 2014, 26, 395009.	0.7	6
10	Supramolecular and Chiral Effects at the Titanyl Phthalocyanine/Ag(100) Hybrid Interface. Journal of Physical Chemistry C, 2014, 118, 5255-5267.	1.5	20
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	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
13	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
14	Tuning of the optical properties of In-rich In[sub x]Ga[sub 1âˆ’x]N (x=0.82âˆ’0.49) alloys by light-ion irradiation at low energy. , 2013, , .		0
15	Identification 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>âˆ’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>N		

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19	Clusters and Magnetic Anchoring Points in (Ga,Fe)N Condensed Magnetic Semiconductors. Physical Review Letters, 2011, 107, 196401.	2.9	23
20	Bound states of the Fe impurity in wurtzite GaN from hybrid density-functional calculations. Physical Review B, 2011, 84, .	1.1	19
21	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
22	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
23	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
24	Local structure of nitrogen-hydrogen complexes in dilute nitrides. Physical Review B, 2009, 79, .	1.1	21
25	Oxygen vacancies and OH species in rutile and anatase TiO2 polymorphs. Catalysis Today, 2009, 144, 177-182.	2.2	67
26	Ab initio Theoretical Investigation of Phthalocyanineâ^'Semiconductor Hybrid Systems. Chemistry of Materials, 2009, 21, 4555-4567.	3.2	27
27	Properties of hydrogen and hydrogenâ€“vacancy complexes in the rutile phase of titanium dioxide. Physical Review B, 2009, 80, .	1.1	60
28	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:msu Physical Review B, 2008, 78, .	1.1	239
29	Short Hydrogen Bonds at the Water/TiO₂ (Anatase) Interface. Journal of Physical Chemistry C, 2008, 112, 13579-13586.	1.5	71
30	Hydrogen and interstitial Mn complexes in MnxGa1â^'xAs dilute magnetic semiconductors. Journal of Physics Condensed Matter, 2008, 20, 125215.	0.7	0
31	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 Physical Review B, 2008, 78, .	1.1	14
32	Theoretical Design of Coupled Organic-Inorganic Systems. Physical Review Letters, 2008, 101, 126805.	2.9	14
33	H-Induced Dangling Bonds in Hâ€“Isoelectronic-Impurity Complexes Formed inGaAs1â^'yNyAlloys. Physical Review Letters, 2007, 98, 206403.	2.9	25
34	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
35	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
36	Theory of hydrogen complexes in Mn xGa1-xAs dilute magnetic semiconductors. Brazilian Journal of Physics, 2006, 36, 245-247.	0.7	1

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37	C2v nitrogen-hydrogen complexes in GaAsN revealed by X-ray Absorption Near-Edge Spectroscopy andab initio simulations. Physica Status Solidi C: Current Topics in Solid State Physics, 2006, 3, 1836-1840.	0.8	0
38	Effects of n-type doping on active Fe sites in ion implanted Fe in InP. Applied Physics Letters, 2006, 88, 251912.	1.5	2
39	Photocatalytic reduction of oxygen molecules at the (100) TiO2 anatase surface. Surface Science, 2005, 577, 59-68.	0.8	21
40	Nitrogen-hydrogen complex inGaAsxN1â^'xrevealed by x-ray absorption spectroscopy. Physical Review B, 2005, 71, .	1.1	56
41	Electron correlation effects on the hydrogen passivation ofMnxGa1â^'xAsdilute magnetic semiconductors. Physical Review B, 2005, 72, .	1.1	10
42	Vibrational spectroscopy of hydrogenatedGaAs1â^'yNy:â€ƒA structure-sensitive test of anH2*(N)model. Physical Review B, 2004, 69, .	1.1	41
43	Structure, electronic properties, and formation mechanisms of hydrogen-nitrogen complexes inGaPyN1â^'yalloys. Physical Review B, 2004, 69, .	1.1	13
44	Hydrogenâ€“nitrogen complexes in GaPyN1â^'y alloys. Physica B: Condensed Matter, 2003, 340-342, 492-495.	1.3	4
45	Local and lattice relaxations in hydrogenatedGaAsyN1â^'yalloys. Physical Review B, 2003, 68, .	1.1	12
46	Lattice relaxation by atomic hydrogen irradiation ofIIIâ^'Nâ^'Vsemiconductor alloys. Physical Review B, 2003, 68, .	1.1	38
47	Nitrogen passivation by atomic hydrogen inGaAsyN1â^'yandInxGa1â^'xAsyN1â^'yalloys. Physical Review B, 2003, 68, .	1.1	34
48	Structure and Passivation Effects of Mono- and Dihydrogen Complexes inGaAsyN1â^'yAlloys. Physical Review Letters, 2002, 89, 216401.	2.9	52
49	Structure and dynamics of small protonated rare-gas clusters using quantum and classical methods. Computer Physics Communications, 2002, 145, 78-96.	3.0	12
50	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
51	Vibrational analysis from linear response theory. Chemical Physics Letters, 2001, 345, 179-182.	1.2	23
52	A novel implicit Newtonâ€“Raphson geometry optimization method for density functional theory calculations. Journal of Chemical Physics, 2001, 115, 636-642.	1.2	15
53	Screening ionic motion in sodalite cages: A dynamical study. Journal of Chemical Physics, 1999, 111, 2761-2769.	1.2	7
54	Competitive shell-filling in protonated helium clusters. Chemical Physics, 1999, 241, 203-212.	0.9	26

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55	Simulating ionic microsolvation: protonated argon clusters. Physical Chemistry Chemical Physics, 1999, 1, 5537-5545.	1.3	4
56	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
57	Charged chromophoric units in protonated rare-gas clusters: A dynamical simulation. Europhysics Letters, 1998, 44, 585-591.	0.7	36
58	Structural and Electronic Properties of Sodalite: An ab Initio Molecular Dynamics Study. The Journal of Physical Chemistry, 1995, 99, 12883-12891.	2.9	40