Guido Fratesi

List of Publications by Year
in descending order

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85	23,759	361413	64796
papers	citations	20 h-index	79 g-index

90	90	90	23331
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Steric hindrance in the on-surface synthesis of diethynyl-linked anthracene polymers. Physical Chemistry Chemical Physics, 2022, 24, 13616-13624.	2.8	2
2	Phthalocyanine reactivity and interaction on the 6H-SiC(0001)-(3 Ã— 3) surface investigated by core-level experiments and simulations. Physical Chemistry Chemical Physics, 2022, 24, 14937-14946.	2.8	2
3	Ordered assembly of non-planar vanadyl-tetraphenylporphyrins on ultra-thin iron oxide. Physical Chemistry Chemical Physics, 2022, 24, 17077-17087.	2.8	3
4	Tailoring the magnetic ordering of the Cr₄O₅/Fe(001) surface via a controlled adsorption of C₆₀ organic molecules. Physical Chemistry Chemical Physics, 2021, 23, 7948-7954.	2.8	1
5	Doping Graphene with Substitutional Mn. ACS Nano, 2021, 15, 5449-5458.	14.6	25
6	Positionâ€Controlled Functionalization of Vacancies in Silicon by Singleâ€Ion Implanted Germanium Atoms. Advanced Functional Materials, 2021, 31, 2011175.	14.9	3
7	Singleâ€Ion Implantation: Positionâ€Controlled Functionalization of Vacancies in Silicon by Singleâ€Ion Implanted Germanium Atoms (Adv. Funct. Mater. 21/2021). Advanced Functional Materials, 2021, 31, 2170151.	14.9	0
8	Twoâ€Dimensional Siliceneâ€“Stanene Heterostructures by Epitaxy. Advanced Functional Materials, 2021, 31, 2102797.	14.9	23
9	Graphdiynes interacting with metal surfaces: first-principles electronic and vibrational properties. 2D Materials, 2021, 8, 044014.	4.4	6
10	Cobalt atoms drive the anchoring of Co-TPP molecules to the oxygen-passivated Fe(0â€¯0â€¯1) surface. Applied Surface Science, 2020, 505, 144213.	6.1	21
11	Nontrivial central-atom dependence in the adsorption of M-TPP molecules (M=Co, Ni, Zn) on Fe(001)-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si108.svg"><mml:mrow><mml:mi>p</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>1</mml:mn><mml:mo>Ã—</mml:mo><mml:mn>1</mml:mn><mml:mo) Tj ETQq1 1 0.78431	6.1	17
12	Coverage-dependent electronic and optical properties of H- or F-passivated Si/Ag(111) from first principles. Physical Review B, 2020, 101, .	3.2	1
13	Ketoâ€“enol tautomerization drives the self-assembly of leucoquinizarin on Au(111). Chemical Communications, 2020, 56, 2833-2836.	4.1	1
14	High Potassium Concentrations Nested in Epitaxial Monolayers of a Flexible Lander-Type Molecule on Ag(111). Journal of Physical Chemistry C, 2020, 124, 4114-4127.	3.1	2
15	Structural, Electronic, and Vibrational Properties of a Two-Dimensional Graphdiyne-like Carbon Nanonetwork Synthesized on Au(111): Implications for the Engineering of sp-sp² Carbon Nanostructures. ACS Applied Nano Materials, 2020, 3, 12178-12187.	5.0	14
16	Energetic Ground State Calculations, Electronic Band Structure at Surfaces. Springer Handbooks, 2020, , 471-498.	0.6	0
17	Effects of the introduction of a chromium oxide monolayer at the C60/Fe(001) interface. Journal of Applied Physics, 2019, 125, 142907.	2.5	3
18	Ab initio study of the structural, electronic, magnetic, and optical properties of silicene nanoribbons. Physical Review B, 2019, 99, .	3.2	15

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19	Scanning tunneling microscopy and Raman spectroscopy of polymeric spâ€“sp² carbon atomic wires synthesized on the Au(111) surface. Nanoscale, 2019, 11, 18191-18200.	5.6	24
20	Lattice Mismatch Drives Spatial Modulation of Corannulene Tilt on Ag(111). Journal of Physical Chemistry C, 2018, 122, 10365-10376.	3.1	8
21	Tuning ultrafast electron injection dynamics at organic-graphene/metal interfaces. Nanoscale, 2018, 10, 8014-8022.	5.6	4
22	Effect of Structural Fluctuations on Elastic Lifetimes of Adsorbate States: Isonicotinic Acid on Rutile(110). Journal of Physical Chemistry C, 2018, 122, 7575-7585.	3.1	7
23	Optical Properties of Free and Si(001)â€Adsorbed Pyrimidinic Nucleobases. Physica Status Solidi (B): Basic Research, 2018, 255, 1700497.	1.5	4
24	Fingerprints of sp1 Hybridized C in the Near-Edge X-ray Absorption Spectra of Surface-Grown Materials. Materials, 2018, 11, 2556.	2.9	5
25	Spectroscopy of Adsorbates and the Role of Interfacial Interactions. , 2018, , 91-104.		0
26	Optical properties of shortest-width zig-zag silicene nano-ribbons: Effects of local fields. Micro and Nano Engineering, 2018, 1, 37-41.	2.9	3
27	Core Level Spectra of Organic Molecules Adsorbed on Graphene. Materials, 2018, 11, 518.	2.9	2
28	Optical properties of organically functionalized silicon surfaces: Uracil-like nucleobases on Si(001). Physical Review B, 2017, 95, .	3.2	11
29	Ultrafast carrier dynamics of epitaxial silicene. , 2017, , .		3
30	Electronic States of Silicene Allotropes on Ag(111). ACS Nano, 2017, 11, 975-982.	14.6	45
31	Chemisorption of Pentacene on Pt(111) with a Little Molecular Distortion. Journal of Physical Chemistry C, 2017, 121, 22797-22805.	3.1	17
32	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
33	Combined spectroscopic and ab initio investigation of monolayer-range Cr oxides on Fe(001): The effect of ordered vacancy superstructure. Physical Review B, 2017, 96, .	3.2	13
34	Fully Atomistic Understanding of the Electronic and Optical Properties of a Prototypical Doped Charge-Transfer Interface. ACS Nano, 2017, 11, 10495-10508.	14.6	20
35	Enhanced Magnetic Hybridization of a Spinterface through Insertion of a Two-Dimensional Magnetic Oxide Layer. Nano Letters, 2017, 17, 7440-7446.	9.1	17
36	Electronic structure and magnetism of strained bcc phases across the fcc to bcc transition in ultrathin Fe films. Physical Review B, 2016, 94, .	3.2	6

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37	Electron coincidence studies of sulfur-overlayers on Cu(001) and Ni(001) surfaces. Journal of Electron Spectroscopy and Related Phenomena, 2016, 211, 32-40.	1.7	6
38	Ultrafast electron injection into photo-excited organic molecules. Physical Chemistry Chemical Physics, 2016, 18, 22140-22145.	2.8	11
39	Electronic transport in B-N substituted bilayer graphene nanojunctions. Physical Review B, 2016, 93, .	3.2	8
40	Femtomagnetism in graphene induced by core level excitation of organic adsorbates. Scientific Reports, 2016, 6, 24603.	3.3	21
41	Effects of Thermal Fluctuations on the Structure, Level Alignment, and Absorption Spectrum of Dye-Sensitized TiO₂: A Comparative Study of Catechol and Isonicotinic Acid on the Anatase (101) and Rutile (110) Surfaces. Journal of Physical Chemistry C, 2016, 120, 3899-3905.	3.1	12
42	Complex Stoichiometry-Dependent Reordering of 3,4,9,10-Perylenetetracarboxylic Dianhydride on Ag(111) upon K Intercalation. ACS Nano, 2016, 10, 2365-2374.	14.6	22
43	Mesoscopic organization of cobalt thin films on clean and oxygen-saturated Fe(001) surfaces. Physical Review B, 2015, 92, .	3.2	16
44	Core-level spectra and molecular deformation in adsorption: V-shaped pentacene on Al(001). Beilstein Journal of Nanotechnology, 2015, 6, 2242-2251.	2.8	9
45	Magnetism in thin Cr films grown on Fe(001)-p(1Ã—1)O: a spin-resolved investigation of single and multi-layers. , 2015, , .		1
46	Optical response and ultrafast carrier dynamics of the silicene-silver interface. Physical Review B, 2015, 92, .	3.2	37
47	The LVV Auger line shape of sulfur on copper studied by Auger photoelectron coincidence spectroscopy. Journal of Physics Condensed Matter, 2015, 27, 085003.	1.8	4
48	TiO2(110) Charge Donation to an Extended Ï€-Conjugated Molecule. Journal of Physical Chemistry Letters, 2015, 6, 308-313.	4.6	20
49	Anchoring and Bending of Pentacene on Aluminum (001). Journal of Physical Chemistry C, 2015, 119, 3624-3633.	3.1	21
50	Graphene magnetism induced by covalent adsorption of aromatic radicals. Physical Chemistry Chemical Physics, 2015, 17, 2210-2215.	2.8	20
51	Multiphoton<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>k</mml:mi></mml:math>-resolved photoemission from gold surface states with 800-nm femtosecond laser pulses. Physical Review B, 2014, 90, .	3.2	22
52	Metallic picene/<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>heterojunctions and the effect of potassium doping. Physical Review B, 2014, 90, .	3.2	0
53	High resolution NEXAFS of perylene and PTCDI: a surface science approach to molecular orbital analysis. Physical Chemistry Chemical Physics, 2014, 16, 14834.	2.8	28
54	Enhanced Atom Mobility on the Surface of a Metastable Film. Physical Review Letters, 2014, 113, 046102.	7.8	22

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55	Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles. Journal of Physical Chemistry C, 2014, 118, 8775-8782.	3.1	12
56	Programming Hierarchical Supramolecular Nanostructures by Molecular Design. Journal of Physical Chemistry C, 2013, 117, 3440-3445.	3.1	20
57	Self-organized chromium oxide monolayers on Fe(001). Physical Review B, 2013, 87, .	3.2	25
58	Azimuthal Dichroism in Near-Edge X-ray Absorption Fine Structure Spectra of Planar Molecules. Journal of Physical Chemistry C, 2013, 117, 6632-6638.	3.1	32
59	Electronic and magnetic properties of bulk Cr tips for scanning tunneling spectroscopy. Physical Review B, 2013, 87, .	3.2	4
60	Conductance calculation of hydrogen molecular junctions between Cu electrodes. Physical Review B, 2013, 87, .	3.2	6
61	Spin-Dependent On-Site Electron Correlations and Localization in Itinerant Ferromagnets. Physical Review Letters, 2012, 109, 126401.	7.8	12
62	Strain effect on local electronic properties of Fe nanoislands grown on Au(111). Physical Review B, 2011, 83, .	3.2	16
63	Unusually Large Magnetic Anisotropy in Electrochemically Deposited Co-Rich Coâ€“Pt Films. ACS Applied Materials & Interfaces, 2011, 3, 1800-1803.	8.0	12
64	Spin Polarized Metastable Helium De-excitation Processes on Metal Surfaces. Journal of Physical Chemistry A, 2011, 115, 8498-8503.	2.5	4
65	First-principles investigation of the early stages of Pd adsorption on Au(111). Journal of Physics Condensed Matter, 2011, 23, 015001.	1.8	8
66	Depolarization and bonding in quasi-one-dimensional Na structures on Cu(001). Physical Review B, 2011, 84, .	3.2	3
67	Adsorption of H2S, HS, S, and H on a stepped Fe(310) surface. European Physical Journal B, 2010, 78, 455-460.	1.5	19
68	Atomic corrugation in scanning tunneling microscopy images of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Fe</mml:mtext><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>001</mml:mn> Physical Review B, 2010, 81, .	3.2	33
69	Charge redistribution in the formation of one-dimensional lithium wires on Cu(001). Physical Review B, 2010, 82, .	3.2	5
70	Short-range lateral interactions and depolarization of Na atoms on Cu surfaces. Journal of Physics Condensed Matter, 2010, 22, 304005.	1.8	4
71	Surface dynamics and friction of K/Cu(001) characterized by helium-3 spin-echo and density functional theory. Physical Review B, 2009, 80, .	3.2	20
72	Dynamics of electron distributions probed by helium scattering. Journal of Physics Condensed Matter, 2009, 21, 264003.	1.8	7

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73	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	1.8	18,183
74	Potential energy surface of alkali atoms adsorbed on Cu(001). Physical Review B, 2009, 80, .	3.2	16
75	Spin-polarized Auger electrons in core-valence-valence decays of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>impurities in metals. Physical Review B, 2009, 79, .	3.2	2
76	Ab initiocalculation of core-valence-valence Auger spectra in closed shell systems. Physical Review B, 2008, 78, .	3.2	14
77	Crucial electronic contributions to measures of surface diffusion by He atom scattering. Physical Review B, 2008, 77, .	3.2	20
78	Spin selectivity by auger-photoelectron coincidence spectroscopy. Journal of Physics: Conference Series, 2008, 100, 072020.	0.4	2
79	Theoretical approaches in adsorption: alkali adatom investigations. Journal of Physics Condensed Matter, 2007, 19, 305005.	1.8	16
80	Hydrogen and Coordination Bonding Supramolecular Structures of Trimesic Acid on Cu(110). Journal of Physical Chemistry A, 2007, 111, 12589-12603.	2.5	118
81	Direct Methane-to-Methanol Conversion:â€‰ Insight from First-Principles Calculations. Journal of Physical Chemistry C, 2007, 111, 17015-17019.	3.1	9
82	Analysis of methane-to-methanol conversion on clean and defective Rh surfaces. Journal of Chemical Physics, 2006, 125, 044701.	3.0	31
83	Methane Dehydrogenation on Rh@Cu(111):Â A First-Principles Study of a Model Catalyst. Journal of the American Chemical Society, 2006, 128, 12448-12454.	13.7	60
84	Templated Growth of Metal-Organic Coordination Chains at Surfaces. Angewandte Chemie - International Edition, 2005, 44, 6142-6145.	13.8	125
85	Many-body method for infinite nonperiodic systems. Physical Review B, 2004, 69, .	3.2	10