

Guido Fratesi

List of Publications by Year in descending order

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85
papers

23,759
citations

361045

20
h-index

64668

79
g-index

90
all docs

90
docs citations

90
times ranked

23331
citing authors

#	ARTICLE	IF	CITATIONS
1	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 395502.	0.7	18,183
2	Advanced capabilities for materials modelling with Quantum ESPRESSO. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 465901.	0.7	4,303
3	Templated Growth of Metal-Organic Coordination Chains at Surfaces. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 6142-6145.	7.2	125
4	Hydrogen and Coordination Bonding Supramolecular Structures of Trimesic Acid on Cu(110). <i>Journal of Physical Chemistry A</i> , 2007, 111, 12589-12603.	1.1	118
5	Methane Dehydrogenation on Rh@Cu(111): A First-Principles Study of a Model Catalyst. <i>Journal of the American Chemical Society</i> , 2006, 128, 12448-12454.	6.6	60
6	Electronic States of Silicene Allotropes on Ag(111). <i>ACS Nano</i> , 2017, 11, 975-982.	7.3	45
7	Optical response and ultrafast carrier dynamics of the silicene-silver interface. <i>Physical Review B</i> , 2015, 92, .	1.1	37
8	Atomic corrugation in scanning tunneling microscopy images of the $Fe(001)$ surface. <i>Physical Review B</i> , 2010, 81, .	1.1	33
9	Azimuthal Dichroism in Near-Edge X-ray Absorption Fine Structure Spectra of Planar Molecules. <i>Journal of Physical Chemistry C</i> , 2013, 117, 6632-6638.	1.5	32
10	Analysis of methane-to-methanol conversion on clean and defective Rh surfaces. <i>Journal of Chemical Physics</i> , 2006, 125, 044701.	1.2	31
11	High resolution NEXAFS of perylene and PTCDI: a surface science approach to molecular orbital analysis. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14834.	1.3	28
12	Self-organized chromium oxide monolayers on Fe(001). <i>Physical Review B</i> , 2013, 87, .	1.1	25
13	Doping Graphene with Substitutional Mn. <i>ACS Nano</i> , 2021, 15, 5449-5458.	7.3	25
14	Scanning tunneling microscopy and Raman spectroscopy of polymeric sp^2 carbon atomic wires synthesized on the Au(111) surface. <i>Nanoscale</i> , 2019, 11, 18191-18200.	2.8	24
15	Two-Dimensional Silicene-Stanene Heterostructures by Epitaxy. <i>Advanced Functional Materials</i> , 2021, 31, 2102797.	7.8	23
16	Multiphoton k -resolved photoemission from gold surface states with 800-nm femtosecond laser pulses. <i>Physical Review B</i> , 2014, 90, .	1.1	22
17	Enhanced Atom Mobility on the Surface of a Metastable Film. <i>Physical Review Letters</i> , 2014, 113, 046102.	2.9	22
18	Complex Stoichiometry-Dependent Reordering of 3,4,9,10-Perylenetetracarboxylic Dianhydride on Ag(111) upon K Intercalation. <i>ACS Nano</i> , 2016, 10, 2365-2374.	7.3	22

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19	Anchoring and Bending of Pentacene on Aluminum (001). Journal of Physical Chemistry C, 2015, 119, 3624-3633.	1.5	21
20	Femtomagnetism in graphene induced by core level excitation of organic adsorbates. Scientific Reports, 2016, 6, 24603.	1.6	21
21	Cobalt atoms drive the anchoring of Co-TPP molecules to the oxygen-passivated Fe(O \hat{e} ⁻ O \hat{e} ⁻) surface. Applied Surface Science, 2020, 505, 144213.	3.1	21
22	Crucial electronic contributions to measures of surface diffusion by He atom scattering. Physical Review B, 2008, 77, .	1.1	20
23	Surface dynamics and friction of K/Cu(001) characterized by helium-3 spin-echo and density functional theory. Physical Review B, 2009, 80, .	1.1	20
24	Programming Hierarchical Supramolecular Nanostructures by Molecular Design. Journal of Physical Chemistry C, 2013, 117, 3440-3445.	1.5	20
25	TiO ₂ (110) Charge Donation to an Extended π -Conjugated Molecule. Journal of Physical Chemistry Letters, 2015, 6, 308-313.	2.1	20
26	Graphene magnetism induced by covalent adsorption of aromatic radicals. Physical Chemistry Chemical Physics, 2015, 17, 2210-2215.	1.3	20
27	Fully Atomistic Understanding of the Electronic and Optical Properties of a Prototypical Doped Charge-Transfer Interface. ACS Nano, 2017, 11, 10495-10508.	7.3	20
28	Adsorption of H ₂ S, HS, S, and H on a stepped Fe(310) surface. European Physical Journal B, 2010, 78, 455-460.	0.6	19
29	Chemisorption of Pentacene on Pt(111) with a Little Molecular Distortion. Journal of Physical Chemistry C, 2017, 121, 22797-22805.	1.5	17
30	Enhanced Magnetic Hybridization of a Spinterface through Insertion of a Two-Dimensional Magnetic Oxide Layer. Nano Letters, 2017, 17, 7440-7446.	4.5	17
31	Nontrivial central-atom dependence in the adsorption of M-TPP molecules (M=Co, Ni, Zn) on Fe(001)- \langle 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> \AA - </mml:mo> <mml:mn> 1 </mml:mn> <mml:mo>)	3.1	17
32	Theoretical approaches in adsorption: alkali adatom investigations. Journal of Physics Condensed Matter, 2007, 19, 305005.	0.7	16
33	Potential energy surface of alkali atoms adsorbed on Cu(001). Physical Review B, 2009, 80, .	1.1	16
34	Strain effect on local electronic properties of Fe nanoislands grown on Au(111). Physical Review B, 2011, 83, .	1.1	16
35	Mesoscopic organization of cobalt thin films on clean and oxygen-saturated Fe(001) surfaces. Physical Review B, 2015, 92, .	1.1	16
36	<i>ab initio</i> study of the structural, electronic, magnetic, and optical properties of silicene nanoribbons. Physical Review B, 2019, 99, .	1.1	15

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37	Ab initio calculation of core-valence-valence Auger spectra in closed shell systems. <i>Physical Review B</i> , 2008, 78, .	1.1	14
38	Structural, Electronic, and Vibrational Properties of a Two-Dimensional Graphdiyne-like Carbon Nanonetwork Synthesized on Au(111): Implications for the Engineering of sp ² Carbon Nanostructures. <i>ACS Applied Nano Materials</i> , 2020, 3, 12178-12187.	2.4	14
39	Combined spectroscopic and <i>ab initio</i> investigation of monolayer-range Cr oxides on Fe(001): The effect of ordered vacancy superstructure. <i>Physical Review B</i> , 2017, 96, .	1.1	13
40	Unusually Large Magnetic Anisotropy in Electrochemically Deposited Co-Rich Co/Pt Films. <i>ACS Applied Materials & Interfaces</i> , 2011, 3, 1800-1803.	4.0	12
41	Spin-Dependent On-Site Electron Correlations and Localization in Itinerant Ferromagnets. <i>Physical Review Letters</i> , 2012, 109, 126401.	2.9	12
42	Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles. <i>Journal of Physical Chemistry C</i> , 2014, 118, 8775-8782.	1.5	12
43	Effects of Thermal Fluctuations on the Structure, Level Alignment, and Absorption Spectrum of Dye-Sensitized TiO ₂ : A Comparative Study of Catechol and Isonicotinic Acid on the Anatase (101) and Rutile (110) Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3899-3905.	1.5	12
44	Ultrafast electron injection into photo-excited organic molecules. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22140-22145.	1.3	11
45	Optical properties of organically functionalized silicon surfaces: Uracil-like nucleobases on Si(001). <i>Physical Review B</i> , 2017, 95, .	1.1	11
46	Many-body method for infinite nonperiodic systems. <i>Physical Review B</i> , 2004, 69, .	1.1	10
47	Direct Methane-to-Methanol Conversion: Insight from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2007, 111, 17015-17019.	1.5	9
48	Core-level spectra and molecular deformation in adsorption: V-shaped pentacene on Al(001). <i>Beilstein Journal of Nanotechnology</i> , 2015, 6, 2242-2251.	1.5	9
49	First-principles investigation of the early stages of Pd adsorption on Au(111). <i>Journal of Physics Condensed Matter</i> , 2011, 23, 015001.	0.7	8
50	Electronic transport in B-N substituted bilayer graphene nanojunctions. <i>Physical Review B</i> , 2016, 93, .	1.1	8
51	Lattice Mismatch Drives Spatial Modulation of Corannulene Tilt on Ag(111). <i>Journal of Physical Chemistry C</i> , 2018, 122, 10365-10376.	1.5	8
52	Dynamics of electron distributions probed by helium scattering. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 264003.	0.7	7
53	Effect of Structural Fluctuations on Elastic Lifetimes of Adsorbate States: Isonicotinic Acid on Rutile(110). <i>Journal of Physical Chemistry C</i> , 2018, 122, 7575-7585.	1.5	7
54	Conductance calculation of hydrogen molecular junctions between Cu electrodes. <i>Physical Review B</i> , 2013, 87, .	1.1	6

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55	Electronic structure and magnetism of strained bcc phases across the fcc to bcc transition in ultrathin Fe films. <i>Physical Review B</i> , 2016, 94, .	1.1	6
56	Electron coincidence studies of sulfur-overlayers on Cu(001) and Ni(001) surfaces. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2016, 211, 32-40.	0.8	6
57	Graphdiynes interacting with metal surfaces: first-principles electronic and vibrational properties. <i>2D Materials</i> , 2021, 8, 044014.	2.0	6
58	Charge redistribution in the formation of one-dimensional lithium wires on Cu(001). <i>Physical Review B</i> , 2010, 82, .	1.1	5
59	Fingerprints of sp ¹ Hybridized C in the Near-Edge X-ray Absorption Spectra of Surface-Grown Materials. <i>Materials</i> , 2018, 11, 2556.	1.3	5
60	Short-range lateral interactions and depolarization of Na atoms on Cu surfaces. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 304005.	0.7	4
61	Spin Polarized Metastable Helium De-excitation Processes on Metal Surfaces. <i>Journal of Physical Chemistry A</i> , 2011, 115, 8498-8503.	1.1	4
62	Electronic and magnetic properties of bulk Cr tips for scanning tunneling spectroscopy. <i>Physical Review B</i> , 2013, 87, .	1.1	4
63	The LW Auger line shape of sulfur on copper studied by Auger photoelectron coincidence spectroscopy. <i>Journal of Physics Condensed Matter</i> , 2015, 27, 085003.	0.7	4
64	Tuning ultrafast electron injection dynamics at organic-graphene/metal interfaces. <i>Nanoscale</i> , 2018, 10, 8014-8022.	2.8	4
65	Optical Properties of Free and Si(001)-Adsorbed Pyrimidinic Nucleobases. <i>Physica Status Solidi (B): Basic Research</i> , 2018, 255, 1700497.	0.7	4
66	Depolarization and bonding in quasi-one-dimensional Na structures on Cu(001). <i>Physical Review B</i> , 2011, 84, .	1.1	3
67	Ultrafast carrier dynamics of epitaxial silicene. , 2017, , .		3
68	Optical properties of shortest-width zig-zag silicene nano-ribbons: Effects of local fields. <i>Micro and Nano Engineering</i> , 2018, 1, 37-41.	1.4	3
69	Effects of the introduction of a chromium oxide monolayer at the C60/Fe(001) interface. <i>Journal of Applied Physics</i> , 2019, 125, 142907.	1.1	3
70	Position-Controlled Functionalization of Vacancies in Silicon by Single-Ion Implanted Germanium Atoms. <i>Advanced Functional Materials</i> , 2021, 31, 2011175.	7.8	3
71	Ordered assembly of non-planar vanadyl-tetraphenylporphyrins on ultra-thin iron oxide. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 17077-17087.	1.3	3
72	Spin selectivity by auger-photoelectron coincidence spectroscopy. <i>Journal of Physics: Conference Series</i> , 2008, 100, 072020.	0.3	2

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73	Spin-polarized Auger electrons in core-valence-valence decays of d impurities in metals. Physical Review B, 2009, 79, .	1.1	2
74	Core Level Spectra of Organic Molecules Adsorbed on Graphene. Materials, 2018, 11, 518.	1.3	2
75	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.	1.5	2
76	Steric hindrance in the on-surface synthesis of diethynyl-linked anthracene polymers. Physical Chemistry Chemical Physics, 2022, 24, 13616-13624.	1.3	2
77	Phthalocyanine reactivity and interaction on the 6H-SiC(0001)-(3 Å ⁻¹) surface investigated by core-level experiments and simulations. Physical Chemistry Chemical Physics, 2022, 24, 14937-14946.	1.3	2
78	Magnetism in thin Cr films grown on Fe(001)-p(1Å ⁻¹)O: a spin-resolved investigation of single and multi-layers. , 2015, , .		1
79	Coverage-dependent electronic and optical properties of H- or F-passivated Si/Ag(111) from first principles. Physical Review B, 2020, 101, .	1.1	1
80	Keto↔enol tautomerization drives the self-assembly of leucoquinizarin on Au(111). Chemical Communications, 2020, 56, 2833-2836.	2.2	1
81	Tailoring the magnetic ordering of the Cr ₄ O ₅ /Fe(001) surface <i>via</i> a controlled adsorption of C ₆₀ organic molecules. Physical Chemistry Chemical Physics, 2021, 23, 7948-7954.	1.3	1
82	Metallic picene/C ₆₀ heterojunctions and the effect of potassium doping. Physical Review B, 2014, 90, .	1.1	0
83	Spectroscopy of Adsorbates and the Role of Interfacial Interactions. , 2018, , 91-104.		0
84	Single-Ion Implantation: Position-Controlled Functionalization of Vacancies in Silicon by Single-Ion Implanted Germanium Atoms (Adv. Funct. Mater. 21/2021). Advanced Functional Materials, 2021, 31, 2170151.	7.8	0
85	Energetic Ground State Calculations, Electronic Band Structure at Surfaces. Springer Handbooks, 2020, , 471-498.	0.3	0