Daniele Stradi

List of Publications by Year
in descending order

30 papers	1,983 citations	394421 19 h-index	501196 28 g-index
31 all docs	31 docs citations	31 times ranked	2631 citing authors

#	Article	IF	Citations
1	QuantumATK: an integrated platform of electronic and atomic-scale modelling tools. Journal of Physics Condensed Matter, 2020, 32, 015901.	1.8	771
2	First-principles Green's-function method for surface calculations: A pseudopotential localized basis set approach. Physical Review B, 2017, 96, .	3.2	211
3	Long-range magnetic order in a purely organic 2D layer adsorbed on epitaxial graphene. Nature Physics, 2013, 9, 368-374.	16.7	158
4	General atomistic approach for modeling metal-semiconductor interfaces using density functional theory and nonequilibrium Green's function. Physical Review B, 2016, 93, .	3.2	137
5	Role of Dispersion Forces in the Structure of Graphene Monolayers on Ru Surfaces. Physical Review Letters, 2011, 106, 186102.	7.8	129
6	Method for determining optimal supercell representation of interfaces. Journal of Physics Condensed Matter, 2017, 29, 185901.	1.8	59
7	Proximity Band Structure and Spin Textures on Both Sides of Topological-Insulator/Ferromagnetic-Metal Interface and Their Charge Transport Probes. Nano Letters, 2017, 17, 5626-5633.	9.1	59
8	Determination of low-strain interfaces via geometric matching. Physical Review B, 2017, 96, .	3.2	47
9	Manipulating the voltage drop in graphene nanojunctions using a gate potential. Physical Chemistry Chemical Physics, 2016, 18, 1025-1031.	2.8	39
10	Organic Covalent Patterning of Nanostructured Graphene with Selectivity at the Atomic Level. Nano Letters, 2016, 16, 355-361.	9.1	36
11	Lattice-matched versus lattice-mismatched models to describe epitaxial monolayer graphene on Ru(0001). Physical Review B, 2013, 88, .	3.2	35
12	Elastic Response of Graphene Nanodomes. ACS Nano, 2013, 7, 2927-2934.	14.6	35
13	Electron localization in epitaxial graphene on Ru(0001) determined by moirÃ© corrugation. Physical Review B, 2012, 85, .	3.2	34
14	Electron-phonon scattering from Green's function transport combined with molecular dynamics: Applications to mobility predictions. Physical Review B, 2017, 95, .	3.2	33
15	A density functional theory study of the manganese-phthalocyanine. Theoretical Chemistry Accounts, 2011, 128, 497-503.	1.4	30
16	Probing the Site-Dependent Kondo Response of Nanostructured Graphene with Organic Molecules. Nano Letters, 2014, 14, 4560-4567.	9.1	24
17	Understanding the self-assembly of TCNQ on Cu(111): a combined study based on scanning tunnelling microscopy experiments and density functional theory simulations. RSC Advances, 2016, 6, 15071-15079.	3.6	22
18	Field Effect in Graphene-Based van der Waals Heterostructures: Stacking Sequence Matters. Nano Letters, 2017, 17, 2660-2666.	9.1	21

#	Article	IF	Citations
19	Controlling the spatial arrangement of organic magnetic anions adsorbed on epitaxial graphene on Ru(0001). Nanoscale, 2014, 6, 15271-15279.	5.6	19
20	Comparative study of the interfaces of graphene and hexagonal boron nitride with silver. Physical Review B, 2016, 94, .	3.2	18
21	Prospective Role of Multicenter Bonding for Efficient and Selective Hydrogen Transport. Physical Review Letters, 2010, 105, 045901.	7.8	17
22	Ordered arrays of metalâ€“organic magnets at surfaces. Journal of Physics Condensed Matter, 2013, 25, 484007.	1.8	16
23	Grazing incidence scattering of vibrationally excited H2 molecules from metal surfaces. Surface Science, 2010, 604, 2031-2035.	1.9	8
24	Atomistic Insight into the Formation of Metal-Graphene One-Dimensional Contacts. Physical Review Applied, 2018, 10, .	3.8	8
25	Schottky barrier lowering due to interface states in 2D heterophase devices. Nanoscale Advances, 2021, 3, 567-574.	4.6	8
26	A theoretical study of a ZnO graphene analogue: adsorption on Ag(111) and hydrogen transport. Journal of Physics Condensed Matter, 2011, 23, 334215.	1.8	5
27	Tunneling spectra of graphene on copper unraveled. Physical Chemistry Chemical Physics, 2016, 18, 17081-17090.	2.8	2
28	Atomistic Modeling Of Nanoscale Ferroelectric Capacitors Using a Density Functional Theory And Non-Equilibrium Greenâ€™s-Function Method. , 2019, , .		1
29	Atomistic approach for modeling metal-semiconductor interfaces. , 2016, , .		0
30	First-principles modeling of SiGe alloys and devices. , 2017, , .		0