Nicolae Atodiresei

List of Publications by Year
in descending order

90 papers	3,526 citations	172386 29 h-index	138417 58 g-index
94 all docs	94 docs citations	94 times ranked	4253 citing authors

#	Article	IF	Citations
1	Interface-engineered templates for molecular spin memory devices. Nature, 2013, 493, 509-513.	13.7	401
2	Design of the Local Spin Polarization at the Organic-Ferromagnetic Interface. Physical Review Letters, 2010, 105, 066601.	2.9	284
3	Graphene on Ir(111): Physisorption with Chemical Modulation. Physical Review Letters, 2011, 107, 036101.	2.9	270
4	Spin- and Energy-Dependent Tunneling through a Single Molecule with Intramolecular Spatial Resolution. Physical Review Letters, 2010, 105, 047204.	2.9	257
5	The mechanism of caesium intercalation of graphene. Nature Communications, 2013, 4, 2772.	5.8	184
6	Atomic-scale magnetism of cobalt-intercalated graphene. Physical Review B, 2013, 87, .	1.1	138
7	Chemical versus van der Waals Interaction: The Role of the Heteroatom in the Flat Absorption of Aromatic Molecules<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">C</mml:mi><mml:mn>6</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">H</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:math>,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant	2.9	132
8	Structure and Growth of Hexagonal Boron Nitride on Ir(111). ACS Nano, 2016, 10, 11012-11026.	7.3	93
9	Magnetic Hardening Induced by Nonmagnetic Organic Molecules. Physical Review Letters, 2013, 111, 106805.	2.9	89
10	Density functional theory with nonlocal correlation: A key to the solution of the CO adsorption puzzle. Physical Review B, 2010, 81, .	1.1	83
11	The Backside of Graphene: Manipulating Adsorption by Intercalation. Nano Letters, 2013, 13, 5013-5019.	4.5	74
12	Accessing 4f-states in single-molecule spintronics. Nature Communications, 2013, 4, 2425.	5.8	71
13	Vacancy complexes with oversized impurities in Si and Ge. Physical Review B, 2005, 71, .	1.1	63
14	Graphene on the Ir(111) surface: from van der Waals to strong bonding. New Journal of Physics, 2010, 12, 113016.	1.2	54
15	Role of the van der Waals interactions on the bonding mechanism of pyridine on Cu(110) and Ag(110) surface: First-principles study. Physical Review B, 2008, 78, .	1.1	52
16	Engineering the magnetic properties of hybrid organic-ferromagnetic interfaces by molecular chemical functionalization. Physical Review B, 2011, 84, .	1.1	52
17	The interplay of structure and spinâ€“orbit strength in the magnetism of metalâ€“benzene sandwiches: from single molecules to infinite wires. Nanotechnology, 2007, 18, 495402.	1.3	49
18	Selfâ€Assembled Nanometerâ€Scale Magnetic Networks on Surfaces: Fundamental Interactions and Functional Properties. Advanced Functional Materials, 2011, 21, 1212-1228.	7.8	48

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19	Tuning the van der Waals Interaction of Graphene with Molecules via Doping. Physical Review Letters, 2015, 115, 236101.	2.9	48
20	Real-space electronic structure calculations with full-potential all-electron precision for transition metals. Physical Review B, 2010, 82, .	1.1	44
21	Long-range magnetic coupling between nanoscale organicâ€“metal hybrids mediated by a nanoskyrmion lattice. Nature Nanotechnology, 2014, 9, 1018-1023.	15.6	44
22	Controlling the Magnetization Direction in Molecules via Their Oxidation State. Physical Review Letters, 2008, 100, 117207.	2.9	42
23	Absence of Edge States in Covalently Bonded Zigzag Edges of Graphene on Ir(111). Advanced Materials, 2013, 25, 1967-1972.	11.1	42
24	JuNoLo â€“ JÃ¼lich nonlocal code for parallel post-processing evaluation of vdW-DF correlation energy. Computer Physics Communications, 2010, 181, 371-379.	3.0	40
25	Chemically functionalized magnetic exchange interactions of hybrid organic-ferromagnetic metal interfaces. Physical Review B, 2015, 91, .	1.1	39
26	Boron-Doped Graphene Nanoribbons: Electronic Structure and Raman Fingerprint. ACS Nano, 2018, 12, 7571-7582.	7.3	38
27	Confinement of Dirac electrons in graphene quantum dots. Physical Review B, 2014, 89, .	1.1	36
28	Semiconductorâ€toâ€Metal Transition and Quasiparticle Renormalization in Doped Graphene Nanoribbons. Advanced Electronic Materials, 2017, 3, 1600490.	2.6	33
29	Sub-molecular modulation of a 4f driven Kondo resonance by surface-induced asymmetry. Nature Communications, 2016, 7, 12785.	5.8	32
30	A Monolayer of Hexagonal Boron Nitride on Ir(111) as a Template for Cluster Superlattices. ACS Nano, 2018, 12, 6871-6880.	7.3	31
31	Interface-assisted spintronics: Tailoring at the molecular scale. MRS Bulletin, 2014, 39, 596-601.	1.7	29
32	Cu-Adatom-Mediated Bonding in Close-Packed Benzoate/Cu(110)-Systems. Langmuir, 2009, 25, 856-864.	1.6	28
33	Magnetic anisotropy energies of metalâ€“benzene sandwiches. International Journal of Quantum Chemistry, 2006, 106, 3208-3213.	1.0	26
34	Ab initioand semi-empirical van der Waals study of grapheneâ€“boron nitride interaction from a molecular point of view. Journal of Physics Condensed Matter, 2012, 24, 424214.	0.7	26
35	Oxygen orders differently under graphene: new superstructures on Ir(111). Nanoscale, 2016, 8, 1932-1943.	2.8	25
36	On-Surface Synthesis of Sandwich Molecular Nanowires on Graphene. Journal of the American Chemical Society, 2017, 139, 9895-9900.	6.6	25

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37	Manipulation of benzene on Cu(110) by dynamic force microscopy: Anab initiostudy. Physical Review B, 2008, 77, .	1.1	23
38	Electronic Mapping of Molecular Orbitals at the Molecule-Metal Interface. Physical Review Letters, 2010, 105, 066801.	2.9	23
39	Identifying Molecular Orbital Energies by Distance-Dependent Transition Voltage Spectroscopy. Journal of Physical Chemistry C, 2011, 115, 15025-15030.	1.5	22
40	Semiempirical van der Waals interactions versusab initiononlocal correlation effects in the thiophene-Cu(111) system. Physical Review B, 2012, 86, .	1.1	22
41	Magnetism in a graphene- 4fâ^'3d hybrid system. Physical Review B, 2017, 95, .	1.1	22
42	Structure and dynamics in liquid bismuth and Bin clusters: A density functional study. Journal of Chemical Physics, 2014, 141, 194503.	1.2	21
43	Molecular induced skyhook effect for magnetic interlayer softening. Physical Review B, 2015, 92, .	1.1	19
44	Rationale for switching to nonlocal functionals in density functional theory. Journal of Physics Condensed Matter, 2012, 24, 424215.	0.7	18
45	Local tunnel magnetoresistance of an iron intercalated graphene-based heterostructure. Journal of Physics Condensed Matter, 2014, 26, 394004.	0.7	18
46	Tuning the surface electronic structure of a Pt₃Ti(111) electro catalyst. Nanoscale, 2016, 8, 13924-13933.	2.8	17
47	Annealing of ion-irradiated hexagonal boron nitride on Ir(111). Physical Review B, 2017, 96, .	1.1	17
48	First-principles investigation of terephthalic acid on Cu(110). Physical Review B, 2007, 76, .	1.1	16
49	Interface-driven formation of a two-dimensional dodecagonal fullerene quasicrystal. Nature Communications, 2017, 8, 15367.	5.8	16
50	Density-functional theory study on the arrangement of adsorbed formate molecules on Cu(110). Physical Review B, 2007, 75, .	1.1	15
51	Hybridisation at the organicâ€“metal interface: a surface-scientific analogue of HÃ¼ckel's rule?. Chemical Communications, 2013, 49, 5993.	2.2	15
52	Spin polarization of Co(0001)/graphene junctions from first principles. Journal of Physics Condensed Matter, 2014, 26, 104204.	0.7	15
53	Spatial variation of geometry, binding, and electronic properties in the moirÃ© superstructure of MoS₂ on Au(111). 2D Materials, 2022, 9, 025003.	2.0	15
54	Cd-vacancy andCd-interstitial complexes inSiandGe. Physical Review B, 2004, 70, .	1.1	14

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55	Magnetic subunits within a single moleculeâ€“surface hybrid. New Journal of Physics, 2017, 19, 053016.	1.2	12
56	Spin-Hybrids: A Single-Molecule Approach to Spintronics. E-Journal of Surface Science and Nanotechnology, 2016, 14, 17-22.	0.1	11
57	Quantum interference effects in molecular spin hybrids. Physical Review B, 2017, 95, .	1.1	11
58	Fine tuning of the electronic structure of Ï€-conjugated molecules for molecular electronics. Nanotechnology, 2011, 22, 145701.	1.3	10
59	STRUCTURAL INTEGRITY OF SINGLE BIS(PHTHALOCYANINATO)-NEODYMIUM(III) MOLECULES ON METAL SURFACES WITH DIFFERENT REACTIVITY. Spin, 2014, 04, 1440007.	0.6	10
60	First-principles insights into the electronic and magnetic structure of hybrid organic-metal interfaces. Journal of Physics Condensed Matter, 2014, 26, 263001.	0.7	10
61	Single Electron Tunneling through a Tailored Arylthio-coronene. Journal of Physical Chemistry C, 2011, 115, 9204-9209.	1.5	9
62	Tuning the electron transport of molecular junctions by chemically functionalizing anchoring groups: First-principles study. Physical Review B, 2012, 85, .	1.1	8
63	Exchange interactions of magnetic surfaces below two-dimensional materials. Physical Review B, 2016, 93, .	1.1	8
64	Designing the Rashba spin texture by adsorption of inorganic molecules. New Journal of Physics, 2017, 19, 043017.	1.2	8
65	Guided Molecular Assembly on a Locally Reactive 2D Material. Advanced Materials, 2017, 29, 1703929.	11.1	7
66	Single-crystal graphene on Ir(110). Physical Review B, 2022, 105, .	1.1	7
67	Creating anisotropic spin-split surface states in momentum space by molecular adsorption. Physical Review B, 2017, 96, .	1.1	6
68	Imaging Individual Molecular-Like Orbitals of a Non-Planar Naphthalene Diimide on Pt(111): A Combined STM and DFT Study. Journal of Physical Chemistry C, 2017, 121, 26916-26924.	1.5	6
69	Ab initio modeling of noncontact atomic force microscopy imaging of benzene on Cu(110) surface. International Journal of Quantum Chemistry, 2008, 108, 2803-2812.	1.0	4
70	Tuning electron transport through molecular junctions by chemical modification of the molecular core: First-principles study. Physical Review B, 2013, 88, .	1.1	4
71	TAILORING FERROMAGNETâ€“MOLECULE INTERFACES: TOWARDS MOLECULAR SPINTRONICS. Spin, 2014, 04, 1440014.	0.6	4
72	Self-assembled monolayers of methylselenolate on the Au(111) surface: A combined STM and DFT study. Surface Science, 2014, 619, 67-70.	0.8	4

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73	Local dimerization and dedimerization of C60 molecules under a tip of scanning tunneling microscope: A first-principles study. Carbon, 2020, 159, 638-647.	5.4	4
74	Magnetic properties of transition metal dichalcogenides-Fe/Ir(111) interfaces from first principles. Physical Review Materials, 2018, 2, .	0.9	4
75	Ab initio study of magnetic nanopatterning of a hybrid transition metal dichalcogenides/Ir(111) system via magnetic clusters. Physical Review Materials, 2019, 3, .	0.9	4
76	Uniaxially Aligned 1D Sandwich-Molecular Wires: Electronic Structure and Magnetism. Journal of Physical Chemistry C, 2022, 126, 3140-3150.	1.5	4
77	Tailoring magnetic anisotropy by graphene-induced selective skyhook effect on 4f-metals. Nanoscale, 2022, 14, 7682-7691.	2.8	4
78	Se intercalation between <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Pt</mml:mi><mml:msub><mml:mi>Se</mml:mi><mml:m and the Pt surface during synthesis of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Pt</mml:mi><mml:msub><mml:mi>Se</mml:mi><mml:m by direct selenization of Pt(111). Physical Review B, 2020, 102, .	1.1	3
79	Magnetism in Molecular Vanadium-Benzene Sandwiches. AIP Conference Proceedings, 2005, , .	0.3	2
80	Arylthio-substituted coronenes as tailored building blocks for molecular electronics. Physical Chemistry Chemical Physics, 2012, 14, 1635-1641.	1.3	2
81	A Short Review on the Magnetic Effects Occurring at Organic Ferromagnetic Interfaces Formed between Benzene-Like Molecules and Graphene with Ferromagnetic Surfaces. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2014, 69, 360-370.	0.7	2
82	Spin-polarized electron transmission through B-doped graphene nanoribbons with Fe functionalization: a first-principles study. New Journal of Physics, 2020, 22, 063022.	1.2	2
83	Corrugated graphene exposes the limits of a widely used ab initio van der Waals DFT functional. Physical Review Materials, 2019, 3, .	0.9	2
84	Selecting the Reaction Path in On-Surface Synthesis through the Electron Chemical Potential in Graphene. Journal of the American Chemical Society, 2022, 144, 11003-11009.	6.6	2
85	AtodireseietÂal.Reply:. Physical Review Letters, 2010, 104, .	2.9	1
86	Systematic chemical functionalization of hybrid moleculeâ€“surface interfaces. Physica Status Solidi (B): Basic Research, 2013, 250, 2267-2276.	0.7	1
87	Impurity-Vacancy Complexes in Si and Ge. Hyperfine Interactions, 2004, 158, 37-40.	0.2	0
88	Protection of one-dimensional Si chains embedded in Pt(111) and protected by a hexagonal boron-nitride monolayer. Surface Science, 2019, 685, 24-33.	0.8	0
89	Impurity-Vacancy Complexes in Si and Ge. , 2005, , 37-40.		0
90	Size-limited high-density nanopore formation in two-dimensional moirÃ© materials. Physical Review B, 2022, 105, .	1.1	0