Andrea Dal Corso

List of Publications by Year
in descending order

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		87888	30922
104	37,303	38	102
papers	citations	h-index	g-index

105	105	105	28618
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	Phonons and related crystal properties from density-functional perturbation theory. Reviews of Modern Physics, 2001, 73, 515-562.	45.6	7,534
3	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
4	Pseudopotentials periodic table: From H to Pu. Computational Materials Science, 2014, 95, 337-350.	3.0	1,196
5	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
6	Ab initiostudy of piezoelectricity and spontaneous polarization in ZnO. Physical Review B, 1994, 50, 10715-10721.	3.2	305
7	Atomic Structure and Vibrational Properties of IcosahedralB4CBoron Carbide. Physical Review Letters, 1999, 83, 3230-3233.	7.8	275
8	String Tension and Stability of Magic Tip-Suspended Nanowires. Science, 2001, 291, 288-290.	12.6	247
9	Spin-orbit coupling with ultrasoft pseudopotentials: Application to Au and Pt. Physical Review B, 2005, 71, .	3.2	238
10	Ab initiocalculation of phonon dispersions in II-VI semiconductors. Physical Review B, 1993, 47, 3588-3592.	3.2	229
11	Generalized-gradient approximations to density-functional theory: A comparative study for atoms and solids. Physical Review B, 1996, 53, 1180-1185.	3.2	228
12	First-principles study of lattice instabilities in ferromagneticNi2MnGa. Physical Review B, 2003, 68, .	3.2	179
13	Ballistic conductance of magnetic Co and Ni nanowires with ultrasoft pseudopotentials. Physical Review B, 2004, 70, .	3.2	178
14	Raman scattering intensities in Î±-quartz: A first-principles investigation. Physical Review B, 2001, 63, .	3.2	173
15	Wannier and Bloch orbital computation of the nonlinear susceptibility. Physical Review B, 1994, 50, 5756-5759.	3.2	121
16	The puzzling stability of monatomic gold wires. Surface Science, 1999, 426, L441-L446.	1.9	120
17	Elastic constants of beryllium: a first-principles investigation. Journal of Physics Condensed Matter, 2016, 28, 075401.	1.8	112
18	Density-functional theory of the nonlinear optical susceptibility: Application to cubic semiconductors. Physical Review B, 1996, 53, 15638-15642.	3.2	103

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19	Phonon dispersions: Performance of the generalized gradient approximation. Physical Review B, 1999, 60, 11427-11431.	3.2	101
20	Density-functional theory of the dielectric constant: Gradient-corrected calculation for silicon. Physical Review B, 1994, 49, 5323-5328.	3.2	87
21	Colossal magnetic anisotropy of monatomic free and deposited platinum nanowires. Nature Nanotechnology, 2008, 3, 22-25.	31.5	87
22	Atomic structure and vibrational properties of icosahedral Î±-boron and B4C boron carbide. Computational Materials Science, 2000, 17, 127-132.	3.0	86
23	Density-functional perturbation theory with ultrasoft pseudopotentials. Physical Review B, 2001, 64, .	3.2	85
24	Ab initiophonon dispersions of Fe and Ni. Physical Review B, 2000, 62, 273-277.	3.2	84
25	Structural and electronic properties of small Cun clusters using generalized-gradient approximations within density functional theory. Journal of Chemical Physics, 1998, 109, 6626-6630.	3.0	78
26	Projector augmented-wave method: Application to relativistic spin-density functional theory. Physical Review B, 2010, 82, .	3.2	78
27	Structural, electronic, and magnetic properties ofFe2SiO4fayalite: Comparison of LDA and GGA results. Physical Review B, 2003, 67, .	3.2	75
28	Density-functional perturbation theory for lattice dynamics with ultrasoft pseudopotentials. Physical Review B, 1997, 56, R11369-R11372.	3.2	71
29	Density-functional theory of macroscopic stress: Gradient-corrected calculations for crystalline Se. Physical Review B, 1994, 50, 4327-4331.	3.2	67
30	Electron-vibration coupling constants in positively charged fullerene. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 2001, 81, 793-812.	0.6	62
31	Ab initiophonon dispersions of transition and noble metals: effects of the exchange and correlation functional. Journal of Physics Condensed Matter, 2013, 25, 145401.	1.8	54
32	Initial Stages of Growth of Copper on MgO(100): A First Principles Study. Physical Review Letters, 1999, 83, 2761-2764.	7.8	49
33	Nonlinear piezoelectricity in CdTe. Physical Review B, 1993, 47, 16252-16256.	3.2	48
34	Adsorption of atomic oxygen on Ag(): a study based on density-functional theory. Surface Science, 2002, 501, 182-190.	1.9	47
35	Electronic properties of ultra-thin aluminum nanowires. Surface Science, 2000, 454-456, 947-951.	1.9	45
36	The Interaction of Ethylene with Perfect and Defective Ag(001) Surfaces. Journal of Physical Chemistry B, 2002, 106, 9839-9846.	2.6	45

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37	Electric fields with ultrasoft pseudo-potentials: Applications to benzene and anthracene. Journal of Chemical Physics, 2004, 120, 9934-9941.	3.0	42
38	CO adsorbed on Cu(001): A comparison between local density approximation and Perdew, Burke, and Ernezerhof generalized gradient approximation. Journal of Chemical Physics, 2001, 114, 483.	3.0	39
39	Ultrasoft pseudopotentials and projector augmented-wave data sets: application to diatomic molecules. Journal of Physics Condensed Matter, 2011, 23, 425501.	1.8	39
40	Complex band structures and decay length in polyethylene chains. Journal of Physics Condensed Matter, 2003, 15, 3731-3740.	1.8	38
41	Magnetic phenomena, spin-orbit effects, and Landauer conductance in Pt nanowire contacts: Density-functional theory calculations. Physical Review B, 2008, 78, .	3.2	38
42	Ballistic conductance and magnetism in short tip suspended Ni nanowires. Physical Review B, 2006, 73, .	3.2	37
43	Density functional perturbation theory for lattice dynamics with fully relativistic ultrasoft pseudopotentials: Application to fcc-Pt and fcc-Au. Physical Review B, 2007, 76, .	3.2	37
44	Selective d-state conduction blocking in nickel nanocontacts. Surface Science, 2002, 507-510, 609-614.	1.9	35
45	Spin-orbit modifications and splittings of deep surface states on clean Au(111). Surface Science, 2008, 602, 893-905.	1.9	34
46	Microscopic structure of the substitutional Al defect in Î± quartz. Physical Review B, 2000, 61, 2621-2625.	3.2	33
47	Sensitivity of the Mott transition to noncubic splitting of the orbital degeneracy: Application toNH3K3C60. Physical Review B, 2002, 66, .	3.2	33
48	Structure and dynamics of oxygen adsorbed on Ag(100) vicinal surfaces. Physical Review B, 2004, 69, .	3.2	32
49	Ab initiocalculations for the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î²</mml:mi></mml:mrow></mml:math>-tin diamond transition in silicon: Comparing theories with experiments. Physical Review B, 2011, 83, .	3.2	31
50	Projector augmented wave method with spin-orbit coupling: Applications to simple solids and zincblende-type semiconductors. Physical Review B, 2012, 86, .	3.2	29
51	Spin-Flop Ordering from Frustrated Ferro- and Antiferromagnetic Interactions: A Combined Theoretical and Experimental Study of aMn/Fe(100)Monolayer. Physical Review Letters, 2005, 95, 117201.	7.8	27
52	Lattice dynamics and thermophysical properties of h.c.p. Os and Ru from the quasi-harmonic approximation. Journal of Physics Condensed Matter, 2017, 29, 395401.	1.8	27
53	Quasi-harmonic temperature dependent elastic constants: applications to silicon, aluminum, and silver. Journal of Physics Condensed Matter, 2020, 32, 315902.	1.8	27
54	Ab initiostudy of the dielectric properties of silicon and gallium arsenide using polarized Wannier functions. Physical Review B, 1998, 58, R7480-R7483.	3.2	26

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55	Density functional perturbation theory within the projector augmented wave method. Physical Review B, 2010, 81, .	3.2	26
56	Clean Ir(111) and Pt(111) electronic surface states: A first-principle fully relativistic investigation. Surface Science, 2015, 637-638, 106-115.	1.9	26
57	First-principles Wannier functions of silicon and gallium arsenide. Physical Review B, 1997, 55, R1909-R1913.	3.2	25
58	Adsorption of ethylene on the Ag() surface. Surface Science, 2002, 507-510, 62-68.	1.9	23
59	Ab initiophonon dispersions of face centered cubic Pb: effects of spinâ€“orbit coupling. Journal of Physics Condensed Matter, 2008, 20, 445202.	1.8	23
60	Substrate reconstruction and electronic surface states: Ag(001). Surface Science, 2001, 486, 65-72.	1.9	20
61	Complex band structure with ultrasoft pseudopotentials: fcc Ni and Ni nanowire. Surface Science, 2003, 532-535, 549-555.	1.9	20
62	DFT Study of a Weakly Ï€-Bonded C2H4on Oxygen-Covered Ag(100). Journal of Physical Chemistry B, 2006, 110, 367-376.	2.6	20
63	Ab initioballistic conductance with spin-orbit coupling: Application to monoatomic wires. Physical Review B, 2006, 74, .	3.2	19
64	Efficient<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>calculat of ballistic electron transport: Application to Au monatomic chains with a CO impurity. Physical Review B, 2013, 87, .	3.2	18
65	Ab initiostudy of CO adsorption on Ni(110): Effects on surface magnetism at low coverage. Physical Review B, 2001, 63, .	3.2	17
66	Oxygen vibrations in Oâ€“Ag(001). Surface Science, 2003, 530, 26-36.	1.9	17
67	Monatomic Au wire with a magnetic Ni impurity: Electronic structure and ballistic conductance. Physical Review B, 2008, 78, .	3.2	17
68	Adsorption of ethylene on stepped Ag() surfaces. Surface Science, 2004, 566-568, 1018-1023.	1.9	16
69	SixC1â^'xO2 alloys: A possible route to stabilize carbon-based silica-like solids?. Solid State Communications, 2007, 144, 273-276.	1.9	16
70	Interaction of a CO molecule with a Pt monatomic wire: Electronic structure and ballistic conductance. Physical Review B, 2008, 78, .	3.2	16
71	Temperature-dependent atomic B factor: an ab initio calculation. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 624-632.	0.1	16
72	Phonons softening in tip-stretched monatomic nanowires. Surface Science, 2003, 532-535, 544-548.	1.9	15

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73	On-surface and subsurface adsorption of oxygen on stepped Ag(210) and Ag(410) surfaces. Surface Science, 2004, 566-568, 1107-1111.	1.9	15
74	Structure and dynamics of the missing-row reconstruction on O/Cu(001) and O/Ag(001). Surface Science, 2006, 600, 5074-5079.	1.9	15
75	Temperature dependent elastic constants and thermodynamic properties of BAs: An ab initio investigation. Journal of Applied Physics, 2020, 127, .	2.5	15
76	Co-adsorption of ethylene and oxygen on the Ag(001) surface. Surface Science, 2003, 532-535, 191-197.	1.9	14
77	Organic molecular crystals in electric fields. Surface Science, 2004, 566-568, 644-649.	1.9	13
78	Meconium microbiome and its relation to neonatal growth and head circumference catch-up in preterm infants. PLoS ONE, 2020, 15, e0238632.	2.5	13
79	Face-dependent Hamaker constants and surface melting or nonmelting of noncubic crystals. Physical Review B, 1993, 47, 9742-9750.	3.2	12
80	On-surface and sub-surface oxygen adsorption on Ag(210): Vibrational properties. Surface Science, 2005, 587, 50-54.	1.9	12
81	Adsorption geometry of benzene on Pd(110): Results of first-principles calculations. Europhysics Letters, 2000, 52, 698-704.	2.0	11
82	Interaction of CO with an Au monatomic chain at different strains: Electronic structure and ballistic transport. Physical Review B, 2012, 85, .	3.2	11
83	Ab initiosimulation of photoemission spectroscopy in solids: Plane-wave pseudopotential approach with applications to normal-emission spectra of Cu(001) and Cu(111). Physical Review B, 2008, 77, .	3.2	9
84	Magnetism-induced ballistic conductance changes in palladium nanocontacts. European Physical Journal B, 2010, 75, 57-64.	1.5	9
85	Effect of stretching on the ballistic conductance of Au nanocontacts in presence of CO: A density functional study. Physical Review B, 2012, 85, .	3.2	9
86	Reliability evaluation of thermophysical properties from first-principles calculations. Journal of Physics Condensed Matter, 2014, 26, 335401.	1.8	9
87	Density functional perturbation theory for lattice dynamics with fully relativistic ultrasoft pseudopotentials: The magnetic case. Physical Review B, 2019, 100, .	3.2	9
88	Lattice dynamics and thermophysical properties of h.c.p. Re and Tc from the quasiâ€harmonic approximation. Physica Status Solidi (B): Basic Research, 2017, 254, .	1.5	8
89	Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method. Physical Review B, 2020, 102, .	3.2	8
90	Quasi-harmonic thermoelasticity of palladium, platinum, copper, and gold from first principles. Journal of Physics Condensed Matter, 2021, 33, 475901.	1.8	8

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91	A Pseudopotential Plane Waves Program (PWSCF) and some Case Studies. Lecture Notes in Quantum Chemistry II, 1996, , 155-178.	0.3	8
92	A first principles study of small Cun clusters based on local-density and generalized-gradient approximations to density functional theory. Computational Materials Science, 1998, 10, 463-467.	3.0	7
93	Vibrational properties of tetrahedral amorphous carbon from first principles. Applied Physics Letters, 1999, 75, 644-646.	3.3	7
94	Spin-polarized electronic surface states of Re(0001): An ab-initio investigation. Surface Science, 2019, 686, 22-29.	1.9	7
95	Coulomb couplings in positively charged fullerene. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 2002, 82, 1611-1647.	0.6	6
96	Lattice dynamics effects on the magnetocrystalline anisotropy energy: Application to MnBi. Physical Review B, 2020, 102, .	3.2	6
97	Ballistic conductance of Ni nanowire with a magnetization reversal. Surface Science, 2004, 566-568, 390-395.	1.9	5
98	Clean Os(0001) electronic surface states: A first-principle fully relativistic investigation. Surface Science, 2018, 671, 17-26.	1.9	3
99	AB INITIO STUDY OF THE STRUCTURAL AND ELECTRONIC PROPERTIES OF ADSORBATES: CO ON Cu(001). Surface Review and Letters, 1997, 04, 885-889.	1.1	2
100	Finite-temperature atomic relaxations: Effect on the temperature-dependent C₄₄ elastic constants of Si and BAs. Journal of Chemical Physics, 0, , .	3.0	2
101	Reply to: â€œThe puzzling stability of monatomic gold wires is the result of small fluctuationsâ€• Surface Science, 2000, 463, 213.	1.9	1
102	Simulation of electron energy loss spectra with the turboEELS and thermo_pw codes. Journal of Physics: Conference Series, 2018, 1136, 012008.	0.4	1
103	AB-INITIO STUDY OF THE STRUCTURE OF Pd(110)-c(4Ã—2)-BENZENE. Surface Review and Letters, 1999, 06, 903-906.	1.1	0
104	Density functional perturbation theory within the projector augmented-waves method: A few benchmarks for molecules and solids. , 2012, , .		0