Andrea Dal Corso

List of Publications by Year
in descending order

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		87723	30848
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	Quasi-harmonic thermoelasticity of palladium, platinum, copper, and gold from first principles. Journal of Physics Condensed Matter, 2021, 33, 475901.	0.7	8
2	Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method. Physical Review B, 2020, 102, .	1.1	8
3	Meconium microbiome and its relation to neonatal growth and head circumference catch-up in preterm infants. PLoS ONE, 2020, 15, e0238632.	1.1	13
4	Lattice dynamics effects on the magnetocrystalline anisotropy energy: Application to MnBi. Physical Review B, 2020, 102, .	1.1	6
5	Temperature dependent elastic constants and thermodynamic properties of BAs: An ab initio investigation. Journal of Applied Physics, 2020, 127, .	1.1	15
6	Quasi-harmonic temperature dependent elastic constants: applications to silicon, aluminum, and silver. Journal of Physics Condensed Matter, 2020, 32, 315902.	0.7	27
7	Density functional perturbation theory for lattice dynamics with fully relativistic ultrasoft pseudopotentials: The magnetic case. Physical Review B, 2019, 100, .	1.1	9
8	Temperature-dependent atomic B factor: an ab initio calculation. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, 624-632.	0.0	16
9	Spin-polarized electronic surface states of Re(0001): An ab-initio investigation. Surface Science, 2019, 686, 22-29.	0.8	7
10	Clean Os(0001) electronic surface states: A first-principle fully relativistic investigation. Surface Science, 2018, 671, 17-26.	0.8	3
11	Simulation of electron energy loss spectra with the turboEELS and thermo_pw codes. Journal of Physics: Conference Series, 2018, 1136, 012008.	0.3	1
12	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, .	0.7	8
13	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	0.7	4,303
14	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.	0.7	27
15	Elastic constants of beryllium: a first-principles investigation. Journal of Physics Condensed Matter, 2016, 28, 075401.	0.7	112
16	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
17	Clean Ir(111) and Pt(111) electronic surface states: A first-principle fully relativistic investigation. Surface Science, 2015, 637-638, 106-115.	0.8	26
18	Pseudopotentials periodic table: From H to Pu. Computational Materials Science, 2014, 95, 337-350.	1.4	1,196

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19	Reliability evaluation of thermophysical properties from first-principles calculations. Journal of Physics Condensed Matter, 2014, 26, 335401.	0.7	9
20	Ab initiophonon dispersions of transition and noble metals: effects of the exchange and correlation functional. Journal of Physics Condensed Matter, 2013, 25, 145401.	0.7	54
21	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, .	1.1	18
22	Density functional perturbation theory within the projector augmented-waves method: A few benchmarks for molecules and solids. , 2012, , .		0
23	Projector augmented wave method with spin-orbit coupling: Applications to simple solids and zincblende-type semiconductors. Physical Review B, 2012, 86, .	1.1	29
24	Interaction of CO with an Au monatomic chain at different strains: Electronic structure and ballistic transport. Physical Review B, 2012, 85, .	1.1	11
25	Effect of stretching on the ballistic conductance of Au nanocontacts in presence of CO: A density functional study. Physical Review B, 2012, 85, .	1.1	9
26	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, .	1.1	31
27	Ultrasoft pseudopotentials and projector augmented-wave data sets: application to diatomic molecules. Journal of Physics Condensed Matter, 2011, 23, 425501.	0.7	39
28	Magnetism-induced ballistic conductance changes in palladium nanocontacts. European Physical Journal B, 2010, 75, 57-64.	0.6	9
29	Density functional perturbation theory within the projector augmented wave method. Physical Review B, 2010, 81, .	1.1	26
30	Projector augmented-wave method: Application to relativistic spin-density functional theory. Physical Review B, 2010, 82, .	1.1	78
31	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	0.7	18,183
32	Spin-orbit modifications and splittings of deep surface states on clean Au(111). Surface Science, 2008, 602, 893-905.	0.8	34
33	Colossal magnetic anisotropy of monatomic free and deposited platinum nanowires. Nature Nanotechnology, 2008, 3, 22-25.	15.6	87
34	Interaction of a CO molecule with a Pt monatomic wire: Electronic structure and ballistic conductance. Physical Review B, 2008, 78, .	1.1	16
35	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, .	1.1	9
36	Ab initiophonon dispersions of face centered cubic Pb: effects of spinâ€“orbit coupling. Journal of Physics Condensed Matter, 2008, 20, 445202.	0.7	23

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37	Magnetic phenomena, spin-orbit effects, and Landauer conductance in Pt nanowire contacts: Density-functional theory calculations. Physical Review B, 2008, 78, .	1.1	38
38	Monatomic Au wire with a magnetic Ni impurity: Electronic structure and ballistic conductance. Physical Review B, 2008, 78, .	1.1	17
39	Density functional perturbation theory for lattice dynamics with fully relativistic ultrasoft pseudopotentials: Application to fcc-Pt and fcc-Au. Physical Review B, 2007, 76, .	1.1	37
40	SixC1â˜'xO2 alloys: A possible route to stabilize carbon-based silica-like solids?. Solid State Communications, 2007, 144, 273-276.	0.9	16
41	Ab initioballistic conductance with spin-orbit coupling: Application to monoatomic wires. Physical Review B, 2006, 74, .	1.1	19
42	DFT Study of a Weakly Ï€-Bonded C2H4on Oxygen-Covered Ag(100). Journal of Physical Chemistry B, 2006, 110, 367-376.	1.2	20
43	Structure and dynamics of the missing-row reconstruction on O/Cu(001) and O/Ag(001). Surface Science, 2006, 600, 5074-5079.	0.8	15
44	Ballistic conductance and magnetism in short tip suspended Ni nanowires. Physical Review B, 2006, 73, .	1.1	37
45	On-surface and sub-surface oxygen adsorption on Ag(210): Vibrational properties. Surface Science, 2005, 587, 50-54.	0.8	12
46	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.	2.9	27
47	Spin-orbit coupling with ultrasoft pseudopotentials: Application to Au and Pt. Physical Review B, 2005, 71, .	1.1	238
48	Structure and dynamics of oxygen adsorbed on Ag(100) vicinal surfaces. Physical Review B, 2004, 69, .	1.1	32
49	Ballistic conductance of Ni nanowire with a magnetization reversal. Surface Science, 2004, 566-568, 390-395.	0.8	5
50	Adsorption of ethylene on stepped Ag() surfaces. Surface Science, 2004, 566-568, 1018-1023.	0.8	16
51	On-surface and subsurface adsorption of oxygen on stepped Ag(210) and Ag(410) surfaces. Surface Science, 2004, 566-568, 1107-1111.	0.8	15
52	Organic molecular crystals in electric fields. Surface Science, 2004, 566-568, 644-649.	0.8	13
53	Electric fields with ultrasoft pseudo-potentials: Applications to benzene and anthracene. Journal of Chemical Physics, 2004, 120, 9934-9941.	1.2	42
54	Ballistic conductance of magnetic Co and Ni nanowires with ultrasoft pseudopotentials. Physical Review B, 2004, 70, .	1.1	178

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55	Phonons softening in tip-stretched monatomic nanowires. Surface Science, 2003, 532-535, 544-548.	0.8	15
56	Oxygen vibrations in Oâ€“Ag(001). Surface Science, 2003, 530, 26-36.	0.8	17
57	Co-adsorption of ethylene and oxygen on the Ag(001) surface. Surface Science, 2003, 532-535, 191-197.	0.8	14
58	Complex band structure with ultrasoft pseudopotentials: fcc Ni and Ni nanowire. Surface Science, 2003, 532-535, 549-555.	0.8	20
59	First-principles study of lattice instabilities in ferromagneticNi2MnGa. Physical Review B, 2003, 68, .	1.1	179
60	Structural, electronic, and magnetic properties ofFe2SiO4fayalite: Comparison of LDA and GGA results. Physical Review B, 2003, 67, .	1.1	75
61	Complex band structures and decay length in polyethylene chains. Journal of Physics Condensed Matter, 2003, 15, 3731-3740.	0.7	38
62	Sensitivity of the Mott transition to noncubic splitting of the orbital degeneracy: Application toNH3K3C60. Physical Review B, 2002, 66, .	1.1	33
63	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
64	Selective d-state conduction blocking in nickel nanocontacts. Surface Science, 2002, 507-510, 609-614.	0.8	35
65	Adsorption of ethylene on the Ag() surface. Surface Science, 2002, 507-510, 62-68.	0.8	23
66	The Interaction of Ethylene with Perfect and Defective Ag(001) Surfaces. Journal of Physical Chemistry B, 2002, 106, 9839-9846.	1.2	45
67	Adsorption of atomic oxygen on Ag(): a study based on density-functional theory. Surface Science, 2002, 501, 182-190.	0.8	47
68	Phonons and related crystal properties from density-functional perturbation theory. Reviews of Modern Physics, 2001, 73, 515-562.	16.4	7,534
69	Substrate reconstruction and electronic surface states: Ag(001). Surface Science, 2001, 486, 65-72.	0.8	20
70	Raman scattering intensities in Î±-quartz: A first-principles investigation. Physical Review B, 2001, 63, .	1.1	173
71	String Tension and Stability of Magic Tip-Suspended Nanowires. Science, 2001, 291, 288-290.	6.0	247
72	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

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73	Density-functional perturbation theory with ultrasoft pseudopotentials. Physical Review B, 2001, 64, .	1.1	85
74	Ab initiostudy of CO adsorption on Ni(110): Effects on surface magnetism at low coverage. Physical Review B, 2001, 63, .	1.1	17
75	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.	1.2	39
76	Adsorption geometry of benzene on Pd(110): Results of first-principles calculations. Europhysics Letters, 2000, 52, 698-704.	0.7	11
77	Microscopic structure of the substitutional Al defect in Î± quartz. Physical Review B, 2000, 61, 2621-2625.	1.1	33
78	Atomic structure and vibrational properties of icosahedral Î±-boron and B4C boron carbide. Computational Materials Science, 2000, 17, 127-132.	1.4	86
79	Electronic properties of ultra-thin aluminum nanowires. Surface Science, 2000, 454-456, 947-951.	0.8	45
80	Reply to: â€œThe puzzling stability of monatomic gold wires is the result of small fluctuationsâ€• Surface Science, 2000, 463, 213.	0.8	1
81	Ab initiophonon dispersions of Fe and Ni. Physical Review B, 2000, 62, 273-277.	1.1	84
82	Vibrational properties of tetrahedral amorphous carbon from first principles. Applied Physics Letters, 1999, 75, 644-646.	1.5	7
83	Initial Stages of Growth of Copper on MgO(100): A First Principles Study. Physical Review Letters, 1999, 83, 2761-2764.	2.9	49
84	AB-INITIO STUDY OF THE STRUCTURE OF Pd(110)-c(4Ã—2)-BENZENE. Surface Review and Letters, 1999, 06, 903-906.	0.5	0
85	Phonon dispersions: Performance of the generalized gradient approximation. Physical Review B, 1999, 60, 11427-11431.	1.1	101
86	The puzzling stability of monatomic gold wires. Surface Science, 1999, 426, L441-L446.	0.8	120
87	Atomic Structure and Vibrational Properties of IcosahedralB4CBoron Carbide. Physical Review Letters, 1999, 83, 3230-3233.	2.9	275
88	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.	1.4	7
89	Structural and electronic properties of small Cun clusters using generalized-gradient approximations within density functional theory. Journal of Chemical Physics, 1998, 109, 6626-6630.	1.2	78
90	Ab initiostudy of the dielectric properties of silicon and gallium arsenide using polarized Wannier functions. Physical Review B, 1998, 58, R7480-R7483.	1.1	26

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91	Density-functional perturbation theory for lattice dynamics with ultrasoft pseudopotentials. Physical Review B, 1997, 56, R11369-R11372.	1.1	71
92	AB INITIO STUDY OF THE STRUCTURAL AND ELECTRONIC PROPERTIES OF ADSORBATES: CO ON Cu(001). Surface Review and Letters, 1997, 04, 885-889.	0.5	2
93	First-principles Wannier functions of silicon and gallium arsenide. Physical Review B, 1997, 55, R1909-R1913.	1.1	25
94	Generalized-gradient approximations to density-functional theory: A comparative study for atoms and solids. Physical Review B, 1996, 53, 1180-1185.	1.1	228
95	Density-functional theory of the nonlinear optical susceptibility: Application to cubic semiconductors. Physical Review B, 1996, 53, 15638-15642.	1.1	103
96	A Pseudopotential Plane Waves Program (PWSCF) and some Case Studies. Lecture Notes in Quantum Chemistry II, 1996, , 155-178.	0.3	8
97	Density-functional theory of the dielectric constant: Gradient-corrected calculation for silicon. Physical Review B, 1994, 49, 5323-5328.	1.1	87
98	Density-functional theory of macroscopic stress: Gradient-corrected calculations for crystalline Se. Physical Review B, 1994, 50, 4327-4331.	1.1	67
99	Wannier and Bloch orbital computation of the nonlinear susceptibility. Physical Review B, 1994, 50, 5756-5759.	1.1	121
100	Ab initiostudy of piezoelectricity and spontaneous polarization in ZnO. Physical Review B, 1994, 50, 10715-10721.	1.1	305
101	Nonlinear piezoelectricity in CdTe. Physical Review B, 1993, 47, 16252-16256.	1.1	48
102	Face-dependent Hamaker constants and surface melting or nonmelting of noncubic crystals. Physical Review B, 1993, 47, 9742-9750.	1.1	12
103	Ab initiocalculation of phonon dispersions in II-VI semiconductors. Physical Review B, 1993, 47, 3588-3592.	1.1	229
104	Finite-temperature atomic relaxations: Effect on the temperature-dependent C₄₄ elastic constants of Si and BAs. Journal of Chemical Physics, 0, , .	1.2	2