

Andrea Dal Corso

List of Publications by Year in descending order

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Version: 2024-02-01

104
papers

37,303
citations

100601

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35168

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all docs

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docs citations

105
times ranked

32630
citing authors

#	ARTICLE	IF	CITATIONS
1	Quasi-harmonic thermoelasticity of palladium, platinum, copper, and gold from first principles. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 475901.	0.7	8
2	Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method. <i>Physical Review B</i> , 2020, 102, .	1.1	8
3	Meconium microbiome and its relation to neonatal growth and head circumference catch-up in preterm infants. <i>PLoS ONE</i> , 2020, 15, e0238632.	1.1	13
4	Lattice dynamics effects on the magnetocrystalline anisotropy energy: Application to MnBi. <i>Physical Review B</i> , 2020, 102, .	1.1	6
5	Temperature dependent elastic constants and thermodynamic properties of BAs: An <i>ab initio</i> investigation. <i>Journal of Applied Physics</i> , 2020, 127, .	1.1	15
6	Quasi-harmonic temperature dependent elastic constants: applications to silicon, aluminum, and silver. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 315902.	0.7	27
7	Density functional perturbation theory for lattice dynamics with fully relativistic ultrasoft pseudopotentials: The magnetic case. <i>Physical Review B</i> , 2019, 100, .	1.1	9
8	Temperature-dependent atomic $\langle B \rangle$ factor: an <i>ab initio</i> calculation. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2019, 75, 624-632.	0.0	16
9	Spin-polarized electronic surface states of Re(0001): An <i>ab-initio</i> investigation. <i>Surface Science</i> , 2019, 686, 22-29.	0.8	7
10	Clean Os(0001) electronic surface states: A first-principle fully relativistic investigation. <i>Surface Science</i> , 2018, 671, 17-26.	0.8	3
11	Simulation of electron energy loss spectra with the turboEELS and thermo_pw codes. <i>Journal of Physics: Conference Series</i> , 2018, 1136, 012008.	0.3	1
12	Lattice dynamics and thermophysical properties of h.c.p. Re and Tc from the quasi-harmonic approximation. <i>Physica Status Solidi (B): Basic Research</i> , 2017, 254, .	0.7	8
13	Advanced capabilities for materials modelling with Quantum ESPRESSO. <i>Journal of Physics Condensed Matter</i> , 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. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 395401.	0.7	27
15	Elastic constants of beryllium: a first-principles investigation. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 075401.	0.7	112
16	Reproducibility in density functional theory calculations of solids. <i>Science</i> , 2016, 351, aad3000.	6.0	1,113
17	Clean Ir(111) and Pt(111) electronic surface states: A first-principle fully relativistic investigation. <i>Surface Science</i> , 2015, 637-638, 106-115.	0.8	26
18	Pseudopotentials periodic table: From H to Pu. <i>Computational Materials Science</i> , 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	<i>Ab initio</i> phonon 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 $\langle \text{DFT} + \text{U} \rangle$ calculations 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	<i>Ab initio</i> calculations for the I^2 -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	<i>Ab initio</i> simulation 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	<i>Ab initio</i> phonon dispersions of face centered cubic Pb: effects of spin-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. <i>Physical Review B</i> , 2008, 78, .	1.1	38
38	Monatomic Au wire with a magnetic Ni impurity: Electronic structure and ballistic conductance. <i>Physical Review B</i> , 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. <i>Physical Review B</i> , 2007, 76, .	1.1	37
40	SixC1 \hat{a} 'xO2 alloys: A possible route to stabilize carbon-based silica-like solids?. <i>Solid State Communications</i> , 2007, 144, 273-276.	0.9	16
41	Ab initioballistic conductance with spin-orbit coupling: Application to monoatomic wires. <i>Physical Review B</i> , 2006, 74, .	1.1	19
42	DFT Study of a Weakly \ddot{e} -Bonded C2H4on Oxygen-Covered Ag(100). <i>Journal of Physical Chemistry B</i> , 2006, 110, 367-376.	1.2	20
43	Structure and dynamics of the missing-row reconstruction on O/Cu(001) and O/Ag(001). <i>Surface Science</i> , 2006, 600, 5074-5079.	0.8	15
44	Ballistic conductance and magnetism in short tip suspended Ni nanowires. <i>Physical Review B</i> , 2006, 73, .	1.1	37
45	On-surface and sub-surface oxygen adsorption on Ag(210): Vibrational properties. <i>Surface Science</i> , 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. <i>Physical Review Letters</i> , 2005, 95, 117201.	2.9	27
47	Spin-orbit coupling with ultrasoft pseudopotentials: Application to Au and Pt. <i>Physical Review B</i> , 2005, 71, .	1.1	238
48	Structure and dynamics of oxygen adsorbed on Ag(100) vicinal surfaces. <i>Physical Review B</i> , 2004, 69, .	1.1	32
49	Ballistic conductance of Ni nanowire with a magnetization reversal. <i>Surface Science</i> , 2004, 566-568, 390-395.	0.8	5
50	Adsorption of ethylene on stepped Ag() surfaces. <i>Surface Science</i> , 2004, 566-568, 1018-1023.	0.8	16
51	On-surface and subsurface adsorption of oxygen on stepped Ag(210) and Ag(410) surfaces. <i>Surface Science</i> , 2004, 566-568, 1107-1111.	0.8	15
52	Organic molecular crystals in electric fields. <i>Surface Science</i> , 2004, 566-568, 644-649.	0.8	13
53	Electric fields with ultrasoft pseudo-potentials: Applications to benzene and anthracene. <i>Journal of Chemical Physics</i> , 2004, 120, 9934-9941.	1.2	42
54	Ballistic conductance of magnetic Co and Ni nanowires with ultrasoft pseudopotentials. <i>Physical Review B</i> , 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 $\text{O}^{\text{ad}}/\text{Ag}(001)$. Surface Science, 2003, 530, 26-36.	0.8	17
57	Co-adsorption of ethylene and oxygen on the $\text{Ag}(001)$ 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 ferromagnetic Ni_2MnGa . Physical Review B, 2003, 68, .	1.1	179
60	Structural, electronic, and magnetic properties of Fe_2SiO_4 fayalite: 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 to $\text{NH}_3\text{K}_3\text{C}_6\text{O}$. 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 $\text{Ag}()$ surface. Surface Science, 2002, 507-510, 62-68.	0.8	23
66	The Interaction of Ethylene with Perfect and Defective $\text{Ag}(001)$ Surfaces. Journal of Physical Chemistry B, 2002, 106, 9839-9846.	1.2	45
67	Adsorption of atomic oxygen on $\text{Ag}()$: 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: $\text{Ag}(001)$. Surface Science, 2001, 486, 65-72.	0.8	20
70	Raman scattering intensities in $\hat{\Gamma}$ -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. <i>Physical Review B</i> , 2001, 64, .	1.1	85
74	Ab initio study of CO adsorption on Ni(110): Effects on surface magnetism at low coverage. <i>Physical Review B</i> , 2001, 63, .	1.1	17
75	CO adsorbed on Cu(001): A comparison between local density approximation and Perdew, Burke, and Ernzerhof generalized gradient approximation. <i>Journal of Chemical Physics</i> , 2001, 114, 483.	1.2	39
76	Adsorption geometry of benzene on Pd(110): Results of first-principles calculations. <i>Europhysics Letters</i> , 2000, 52, 698-704.	0.7	11
77	Microscopic structure of the substitutional Al defect in $\hat{1}\pm$ quartz. <i>Physical Review B</i> , 2000, 61, 2621-2625.	1.1	33
78	Atomic structure and vibrational properties of icosahedral $\hat{1}\pm$ -boron and B ₄ C boron carbide. <i>Computational Materials Science</i> , 2000, 17, 127-132.	1.4	86
79	Electronic properties of ultra-thin aluminum nanowires. <i>Surface Science</i> , 2000, 454-456, 947-951.	0.8	45
80	Reply to: "The puzzling stability of monatomic gold wires is the result of small fluctuations". <i>Surface Science</i> , 2000, 463, 213.	0.8	1
81	Ab initio phonon dispersions of Fe and Ni. <i>Physical Review B</i> , 2000, 62, 273-277.	1.1	84
82	Vibrational properties of tetrahedral amorphous carbon from first principles. <i>Applied Physics Letters</i> , 1999, 75, 644-646.	1.5	7
83	Initial Stages of Growth of Copper on MgO(100): A First Principles Study. <i>Physical Review Letters</i> , 1999, 83, 2761-2764.	2.9	49
84	AB-INITIO STUDY OF THE STRUCTURE OF Pd(110)-c(4 \times 2)-BENZENE. <i>Surface Review and Letters</i> , 1999, 06, 903-906.	0.5	0
85	Phonon dispersions: Performance of the generalized gradient approximation. <i>Physical Review B</i> , 1999, 60, 11427-11431.	1.1	101
86	The puzzling stability of monatomic gold wires. <i>Surface Science</i> , 1999, 426, L441-L446.	0.8	120
87	Atomic Structure and Vibrational Properties of Icosahedral B ₄ C Boron Carbide. <i>Physical Review Letters</i> , 1999, 83, 3230-3233.	2.9	275
88	A first principles study of small Cu _n clusters based on local-density and generalized-gradient approximations to density functional theory. <i>Computational Materials Science</i> , 1998, 10, 463-467.	1.4	7
89	Structural and electronic properties of small Cu _n clusters using generalized-gradient approximations within density functional theory. <i>Journal of Chemical Physics</i> , 1998, 109, 6626-6630.	1.2	78
90	Ab initio study of the dielectric properties of silicon and gallium arsenide using polarized Wannier functions. <i>Physical Review B</i> , 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 initio study 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 initio calculation 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 C_{44} elastic constants of Si and BAs. Journal of Chemical Physics, 0, , .	1.2	2