Alex Antonelli

List of Publications by Year
in descending order

95	2,224	279798	233421
papers	citations	23 h-index	45 g-index

95	95	95	1911
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Nitrogen and potentialn-type dopants in diamond. Physical Review Letters, 1991, 66, 2010-2013.	7.8	342
2	Divacancies in Graphene and Carbon Nanotubes. Nano Letters, 2007, 7, 2459-2462.	9.1	175
3	Mechanism of self-diffusion in diamond. Physical Review Letters, 1988, 61, 2689-2692.	7.8	162
4	Pressure effects on self-diffusion in silicon. Physical Review B, 1989, 40, 10643-10646.	3.2	120
5	Optimized Free-Energy Evaluation Using a Single Reversible-Scaling Simulation. Physical Review Letters, 1999, 83, 3973-3977.	7.8	100
6	Vacancy in Silicon Revisited: Structure and Pressure Effects. Physical Review Letters, 1998, 81, 2088-2091.	7.8	64
7	Einstein crystal as a reference system in free energy estimation using adiabatic switching. Physical Review E, 1996, 53, 465-474.	2.1	61
8	Adiabatic switching applied to realistic crystalline solids: Vacancy-formation free energy in copper. Physical Review B, 1997, 55, 735-744.	3.2	50
9	Single-simulation determination of phase boundaries: A dynamic Clausiusâ€“Clapeyron integration method. Journal of Chemical Physics, 2001, 115, 11025-11035.	3.0	49
10	Theory of native defects, doping and diffusion in diamond and silicon carbide. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1992, 11, 265-272.	3.5	48
11	Impurity incorporation and doping of diamond. Physica B: Condensed Matter, 1993, 185, 144-149.	2.7	45
12	Insights into the thermoelectric properties of SnSe from ab initio calculations. Physical Chemistry Chemical Physics, 2017, 19, 12804-12815.	2.8	42
13	Transitions between disordered phases in supercooled liquid silicon. Journal of Chemical Physics, 2004, 120, 11672-11677.	3.0	40
14	Stabilization of substitutional Mn in silicon-based semiconductors. Physical Review B, 2004, 70, .	3.2	38
15	Orientational Defects in Ice Ih: An Interpretation of Electrical Conductivity Measurements. Physical Review Letters, 2006, 96, 075501.	7.8	35
16	CrystallineAs2Se3: Electronic and geometric structure. Physical Review B, 1986, 34, 4059-4073.	3.2	34
17	Direct measurement of heavy-hole exciton transport in type-II GaAs/AlAs superlattices. Physical Review Letters, 1993, 71, 3717-3720.	7.8	33
18	Point defect interactions with extended defects in semiconductors. Physical Review B, 1999, 60, 4711-4714.	3.2	32

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19	Bundling up Carbon Nanotubes through Wigner Defects. Nano Letters, 2005, 5, 1045-1049.	9.1	32
20	Thermal stability of supported metal clusters. Physical Review B, 1993, 48, 8263-8266.	3.2	29
21	Electronic properties of a cluster-based solid form of carbon:C28hyperdiamond. Physical Review B, 1994, 49, 8446-8453.	3.2	29
22	Theoretical evidence for a first-order liquid-liquid phase transition in gallium. Journal of Chemical Physics, 2009, 130, 221101.	3.0	28
23	Thermal stability and structural transition in Be microclusters. Physical Review B, 1992, 46, 7841-7845.	3.2	24
24	Finite-temperature molecular-dynamics study of unstable stacking fault free energies in silicon. Physical Review B, 1998, 58, 12555-12558.	3.2	23
25	Dislocation core properties in semiconductors. Solid State Communications, 2001, 118, 651-655.	1.9	23
26	Structure and Energetics of Molecular Point Defects in Icelh. Physical Review Letters, 2006, 97, 155501.	7.8	22
27	Path integral calculation of free energies: Quantum effects on the melting temperature of neon. Journal of Chemical Physics, 2008, 129, 064110.	3.0	22
28	Modeling equilibrium concentrations of Bjerrum and molecular point defects and their complexes in ice Ih. Journal of Chemical Physics, 2008, 128, 164502.	3.0	22
29	Size dependence of the lattice parameter for Pd clusters: A molecular-dynamics study. Physical Review B, 1996, 54, 17057-17060.	3.2	20
30	Atomistic prediction of equilibrium vacancy concentrations inNi3Al. Physical Review B, 2002, 66, .	3.2	20
31	Effects of extended defects on the properties of intrinsic and extrinsic point defects in silicon. Physica B: Condensed Matter, 1999, 273-274, 473-475.	2.7	19
32	Efficient free-energy calculations by the simulation of nonequilibrium processes. Computing in Science and Engineering, 2000, 2, 88-96.	1.2	18
33	Temperature effects on dislocation core energies in silicon and germanium. Physical Review B, 2003, 67, .	3.2	18
34	N-Type Doping and Diffusion of Impurities in Diamond. Materials Research Society Symposia Proceedings, 1989, 162, 315.	0.1	17
35	On the Trapping of Bjerrum Defects in Ice I_h:â€‰ The Case of the Molecular Vacancy. Journal of Physical Chemistry B, 2007, 111, 12537-12542.	2.6	17
36	Pressure and Strain Effects on Diffusion. Materials Research Society Symposia Proceedings, 1989, 163, 523.	0.1	16

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37	Dislocation core reconstruction in zinc-blende semiconductors. Journal of Physics Condensed Matter, 2000, 12, 10039-10044.	1.8	16
38	Diffusion of Pd clusters on Pd(111) surfaces: a molecular dynamics study. Surface Science, 2000, 452, 239-246.	1.9	16
39	Dynamics near a liquid-liquid phase transition in a non-tetrahedral liquid: The case of gallium. Journal of Chemical Physics, 2012, 136, 064513.	3.0	16
40	Ultralow and anisotropic thermal conductivity in semiconductor As₂Se₃. Physical Chemistry Chemical Physics, 2018, 20, 1809-1816.	2.8	16
41	New insight into the electronic structure of aAs2Se3. Physical Review B, 1986, 33, 2968-2971.	3.2	14
42	Quasiparticle bands and optical properties of SnSe from an ab initio approach. Computational Materials Science, 2018, 152, 107-112.	3.0	14
43	Free energy of the concerted-exchange mechanism for self-diffusion in silicon. Physical Review B, 1996, 53, 1310-1314.	3.2	13
44	Interaction of As impurities with 30Â° partial dislocations in Si: An ab initio investigation. Journal of Applied Physics, 2002, 91, 5892-5895.	2.5	13
45	Investigating charge carrier scattering processes in anisotropic semiconductors through first-principles calculations: the case of p-type SnSe. Physical Chemistry Chemical Physics, 2021, 23, 900-913.	2.8	13
46	Binding energies of excitons in ionic quantum well structures. Semiconductor Science and Technology, 1996, 11, 74-79.	2.0	11
47	Vacancy-like defects in a-Si: a first principles study. Journal of Non-Crystalline Solids, 2004, 338-340, 400-402.	3.1	11
48	Thermodynamics of type-I and type-II Si clathrates at zero pressure: Monte Carlo simulations. Physical Review B, 2006, 74, .	3.2	11
49	Pressure effects on the transitions between disordered phases in supercooled liquid silicon. Journal of Chemical Physics, 2011, 135, 204508.	3.0	11
50	Estimating carrier relaxation times in the Ba₈Ga₁₆Ge₃₀ clathrate in the extrinsic regime. Physical Chemistry Chemical Physics, 2017, 19, 3010-3018.	2.8	11
51	First-principles prediction of a metastable crystalline phase of Ga with<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>C</mml:mi><mml:mi>m</mml:mi><mml:mi>c</mml:mi><mml:mi>m</mml:mi></mml:mrow> Physical Review B, 2009, 80, .	3.2	10
52	Efficient method to include nuclear quantum effects in the determination of phase boundaries. Journal of Chemical Physics, 2012, 137, 034114.	3.0	10
53	CrystallineAs2Se3: Optical properties. Physical Review B, 1986, 34, 8718-8727.	3.2	9
54	Theoretical study of cubic structures based on fullerene carbon clusters:C28C and (C28)2. Physical Review B, 1995, 52, 2125-2130.	3.2	9

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55	Stacking-Fault Based Microscopic Model for Platelets in Diamond. Physical Review Letters, 2004, 93, 265502.	7.8	9
56	Theoretical investigation of a Mn-dopedSiâ•Geheterostructure. Physical Review B, 2007, 75, .	3.2	9
57	Boosting the efficiency of ab initio electron-phonon coupling calculations through dual interpolation. Physical Review B, 2020, 102, .	3.2	9
58	Revisiting dynamics near a liquid-liquid phase transition in Si and Ga: The fragile-to-strong transition. Journal of Chemical Physics, 2013, 139, 224504.	3.0	8
59	Stochastic sampling of the isothermal-isobaric ensemble: Phase diagram of crystalline solids from molecular dynamics simulation. Journal of Chemical Physics, 2018, 149, 064114.	3.0	8
60	Computational study of configurational and vibrational contributions to the thermodynamics of substitutional alloys: The case of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ni</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub	3.2	7
61	Microscopic origin of the high thermoelectric figure of merit of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math> -doped SnSe. Physical Review B, 2021, 104, .	3.2	7
62	Splitting up entropy into vibrational and configurational contributions in bulk metallic glasses: A thermodynamic approach. Physical Review Research, 2020, 2, .	3.6	7
63	Arsenic segregation, pairing and mobility on the cores of partial dislocations in silicon. Journal of Physics Condensed Matter, 2002, 14, 12761-12765.	1.8	6
64	On the nature of the solvated electron in ice I_h. Physical Chemistry Chemical Physics, 2016, 18, 4652-4658.	2.8	6
65	Revisiting the fragile-to-strong crossover in metallic glass-forming liquids: Application to <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cu</mml:mi><mml:mi>x</mml:mi></mml:msub	2.4	6
66	Out-of-plane thermoelectric performance for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math> -doped GeSe. Physical Review B, 2022, 105, .	3.2	6
67	Interplanar relaxation at the (0001) surface of Be. Surface Science, 1993, 289, L614-L616.	1.9	4
68	Segregation of dopant atoms on extended defects in semiconductors. Physica B: Condensed Matter, 2001, 302-303, 403-407.	2.7	4
69	Nonphysical thermodynamical phases in L12 intermetallic alloys from semiempirical tight-binding potentials. Computational Materials Science, 2008, 42, 68-73.	3.0	4
70	Hosting of La3+ guest ions in type-I Ge clathrates: A first-principles characterization for thermoelectric applications. Computational Materials Science, 2016, 122, 46-56.	3.0	4
71	Reversible scaling: Optimized free-energy determination using atomistic simulation techniques. Journal of Computer-Aided Materials Design, 1999, 6, 349-353.	0.7	3
72	The energetics of dislocation cores in semiconductors and their role on dislocation mobility. Physica B: Condensed Matter, 2001, 302-303, 398-402.	2.7	3

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73	Nonequilibrium Free Energy Methods Applied to Magnetic Systems: The Degenerate Ising Model. Journal of Statistical Physics, 2019, 175, 1006-1021.	1.2	3
74	Non-equilibrium free-energy calculation of phase-boundaries using LAMMPS. Computational Materials Science, 2022, 207, 111275.	3.0	3
75	Analysis of pseudo-Jahn-Teller instability: O, S, andNâ˜in silicon. Physical Review B, 1987, 35, 6450-6453.	3.2	2
76	Pressure-induced transformations in amorphous silicon: A computational study. Journal of Applied Physics, 2014, 115, 063504.	2.5	2
77	Effects of the local electron speed on the exchange-correlation phenomena. Lettere Al Nuovo Cimento Rivista Internazionale Della SocietÃ Italiana Di Fisica, 1979, 25, 485-488.	0.4	1
78	Ground state properties of crystalline As2Se3. Journal of Non-Crystalline Solids, 1985, 77-78, 95-98.	3.1	1
79	Theory of Doping of Diamond. Materials Research Society Symposia Proceedings, 1992, 242, 323.	0.1	1
80	Interplanar relaxation at the (0001) surface of Be. Surface Science Letters, 1993, 289, L614-L616.	0.1	1
81	Binding energies of excitons in ionic quantum well structures. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1995, 17, 1343-1347.	0.4	1
82	Optical studies of heterointerfacial growth interrupts in type-II GaAs/AlAs superlattices by time resolved photoluminescence imaging. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1995, 13, 1760.	1.6	1
83	Crystalline Structure Around the Single Vacancy in Silicon: Formation Volume and Stress Effects. Materials Research Society Symposia Proceedings, 1998, 527, 377.	0.1	1
84	Dopant interaction with a dislocation in silicon: local and non-local effects. Physica B: Condensed Matter, 2001, 308-310, 470-473.	2.7	1
85	Miranda, Antonelli, and Nunes Reply:. Physical Review Letters, 2005, 95, .	7.8	1
86	The Calculation of Free-Energiesin Semiconductors: Defects, Transitionsand Phase Diagrams. , 0, , 115-140.		1
87	Polyamorphism in tetrahedral substances: Similarities between silicon and ice. Journal of Chemical Physics, 2015, 143, 034501.	3.0	1
88	Native Defects in Diamond, Sic, and Si: Energetics and Self-Diffusion. Materials Research Society Symposia Proceedings, 1988, 141, 249.	0.1	0
89	Many-electron treatment for chalcogen complexes in silicon. Semiconductor Science and Technology, 1990, 5, 196-199.	2.0	0
90	Point Defect Interactions with Extended Defects in Silicon. Materials Research Society Symposia Proceedings, 1998, 538, 419.	0.1	0

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91	Unstable Stacking Fault Free Energies in Silicon through Empirical Modeling. Materials Research Society Symposia Proceedings, 1998, 539, 175.	0.1	0
92	Effective Determination of Coexistence Curves using Reversible-Scaling Molecular Dynamics Simulations. Materials Research Society Symposia Proceedings, 2000, 653, .	0.1	0
93	Thermodynamics of supercooled liquid silicon and its glass transition. Materials Research Society Symposia Proceedings, 2002, 754, 1.	0.1	0
94	Effective Determination of Coexistence Curves using Reversible-Scaling Molecular Dynamics Simulations. Materials Research Society Symposia Proceedings, 2000, 653, 1.	0.1	0
95	Impurity incorporation and doping of diamond. , 1993, , 144-149.		0