

Raffaele Resta

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137
papers

9,768
citations

47
h-index

97
g-index

145
ext. papers

10,826
ext. citations

4.3
avg, IF

6.54
L-index

#	Paper	IF	Citations
137	Macroscopic polarization in crystalline dielectrics: the geometric phase approach. <i>Reviews of Modern Physics</i> , 1994 , 66, 899-915	40.5	1651
136	Band offsets in lattice-matched heterojunctions: A model and first-principles calculations for GaAs/AlAs. <i>Physical Review Letters</i> , 1988 , 61, 734-737	7.4	465
135	Quantum-Mechanical Position Operator in Extended Systems. <i>Physical Review Letters</i> , 1998 , 80, 1800-1803	7.4	420
134	Ab initio calculation of the macroscopic dielectric constant in silicon. <i>Physical Review B</i> , 1986 , 33, 7017-7021	7.4	406
133	Theory of the electric polarization in crystals. <i>Ferroelectrics</i> , 1992 , 136, 51-55	0.6	319
132	Electron Localization in the Insulating State. <i>Physical Review Letters</i> , 1999 , 82, 370-373	7.4	315
131	Towards a quantum theory of polarization in ferroelectrics: The case of KNbO ₃ . <i>Physical Review Letters</i> , 1993 , 70, 1010-1013	7.4	269
130	Ab initio study of piezoelectricity and spontaneous polarization in ZnO. <i>Physical Review B</i> , 1994 , 50, 10715-10726	7.4	265
129	Thomas-Fermi dielectric screening in semiconductors. <i>Physical Review B</i> , 1977 , 16, 2717-2722	3.3	231
128	Orbital magnetization in periodic insulators. <i>Physical Review Letters</i> , 2005 , 95, 137205	7.4	227
127	Ab initio calculation of phonon dispersions in II-VI semiconductors. <i>Physical Review B</i> , 1993 , 47, 3588-3592	3.3	196
126	Manifestations of Berry's phase in molecules and condensed matter. <i>Journal of Physics Condensed Matter</i> , 2000 , 12, R107-R143	1.8	177
125	Theory of Polarization: A Modern Approach 2007 , 31-68		176
124	Valence-band offsets at strained Si/Ge interfaces. <i>Physical Review B</i> , 1991 , 44, 5572-5579	3.3	168
123	Piezoelectric properties of III-V semiconductors from first-principles linear-response theory. <i>Physical Review Letters</i> , 1989 , 62, 2853-2856	7.4	161
122	Role of covalent bonding in the polarization of perovskite oxides: The case of KNbO ₃ . <i>Physical Review B</i> , 1994 , 50, 8911-8914	3.3	155
121	Why are insulators insulating and metals conducting?. <i>Journal of Physics Condensed Matter</i> , 2002 , 14, R625-R656	1.8	142

120	Macroscopic Electric Polarization as a Geometric Quantum Phase. <i>Europhysics Letters</i> , 1993 , 22, 133-138	1.6	139
119	Dipolar correlations and the dielectric permittivity of water. <i>Physical Review Letters</i> , 2007 , 98, 247401	7.4	138
118	Spontaneous polarization as a Berry phase of the Hartree-Fock wave function: The case of KNbO ₃ . <i>Physical Review B</i> , 1997 , 56, 10105-10114	3.3	130
117	Self-consistent theory of electronic states and dielectric response in semiconductors. <i>Physical Review B</i> , 1986 , 34, 7146-7157	3.3	125
116	Local interface composition and band discontinuities in heterovalent heterostructures. <i>Physical Review Letters</i> , 1994 , 72, 294-297	7.4	122
115	Intermolecular dynamical charge fluctuations in water: a signature of the H-bond network. <i>Physical Review Letters</i> , 2005 , 95, 187401	7.4	121
114	The insulating state of matter: a geometrical theory. <i>European Physical Journal B</i> , 2011 , 79, 121-137	1.2	112
113	Towards a bulk theory of flexoelectricity. <i>Physical Review Letters</i> , 2010 , 105, 127601	7.4	109
112	Electrical polarization and orbital magnetization: the modern theories. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 123201	1.8	106
111	Electron localization in the insulating state: Application to crystalline semiconductors. <i>Physical Review B</i> , 2001 , 64,	3.3	106
110	Ab initio study of the spontaneous polarization of pyroelectric BeO. <i>Physical Review Letters</i> , 1990 , 64, 1777-1780	7.4	101
109	Tuning band offsets at semiconductor interfaces by intralayer deposition. <i>Physical Review B</i> , 1991 , 43, 7347-7350	3.3	98
108	External Fields in the Self-Consistent Theory of Electronic States: A New Method for Direct Evaluation of Macroscopic and Microscopic Dielectric Response. <i>Physical Review Letters</i> , 1983 , 51, 686-689	7.4	90
107	Noncubic Behavior of Antiferromagnetic Transition-Metal Monoxides with the Rocksalt Structure. <i>Physical Review Letters</i> , 1999 , 82, 430-433	7.4	81
106	Many-body effects on polarization and dynamical charges in a partly covalent polar insulator. <i>Physical Review Letters</i> , 1995 , 74, 4738-4741	7.4	81
105	Density-functional theory of the dielectric constant: Gradient-corrected calculation for silicon. <i>Physical Review B</i> , 1994 , 49, 5323-5328	3.3	81
104	Mapping topological order in coordinate space. <i>Physical Review B</i> , 2011 , 84,	3.3	79
103	Nonlinear impurity screening in semiconductors. <i>Physical Review B</i> , 1978 , 17, 3239-3242	3.3	64

102	Shallow-Deep Instabilities of Donor Impurity Levels and Excitons in Many-Valley Semiconductors. <i>Physical Review Letters</i> , 1980 , 44, 1340-1344	7.4	63
101	Density-functional theory of macroscopic stress: Gradient-corrected calculations for crystalline Se. <i>Physical Review B</i> , 1994 , 50, 4327-4331	3.3	61
100	Role of dipolar correlations in the infrared spectra of water and ice. <i>Physical Review B</i> , 2008 , 77,	3.3	59
99	Hartree-Fock studies of surface properties of BaTiO ₃ . <i>Physical Review B</i> , 1999 , 60, 2697-2703	3.3	57
98	Ab initio calculation of the low-frequency Raman cross section in silicon. <i>Physical Review B</i> , 1986 , 33, 5969-5971	3.3	55
97	Dielectric matrices and local fields in polar semiconductors. <i>Physical Review B</i> , 1981 , 23, 6615-6624	3.3	54
96	Kohn's theory of the insulating state: a quantum-chemistry viewpoint. <i>Journal of Chemical Physics</i> , 2006 , 124, 104104	3.9	53
95	Microscopic atomic structure and stability of Si-Ge solid solutions. <i>Physical Review B</i> , 1988 , 37, 1308-1314	3.3	53
94	A converse approach to the calculation of NMR shielding tensors. <i>Journal of Chemical Physics</i> , 2009 , 131, 101101	3.9	49
93	Electron localization at metal surfaces. <i>Surface Science</i> , 2000 , 450, 126-132	1.8	48
92	Microscopic capacitors and neutral interfaces in III-V/IV/III-V semiconductor heterostructures. <i>Physical Review Letters</i> , 1992 , 69, 1283-1286	7.4	48
91	Real-space force constants for lattice dynamics in silicon and germanium in the adiabatic bond-charge model. <i>Physical Review B</i> , 1986 , 34, 7140-7145	3.3	47
90	Large binding due to dispersive screening and Bloch function interference in many-valley semiconductors. <i>Solid State Communications</i> , 1979 , 29, 275-277	1.6	47
89	Absolute deformation potentials in semiconductors. <i>Physical Review B</i> , 1990 , 41, 12358-12361	3.3	46
88	Nonstructural theory of the exciton states in solid rare gases. <i>Physical Review B</i> , 1978 , 18, 696-701	3.3	45
87	Ab initio simulation of the properties of ferroelectric materials. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2003 , 11, R69-R96	2	44
86	Nonlinear piezoelectricity in CdTe. <i>Physical Review B</i> , 1993 , 47, 16252-16256	3.3	41
85	Electronic structure of InP/Ga _{0.47} In _{0.53} As interfaces. <i>Physical Review B</i> , 1990 , 41, 12106-12110	3.3	38

84	Electron localization in the quantum Hall regime. <i>Physical Review Letters</i> , 2005 , 95, 196805	7.4	35
83	Dynamical monopoles and dipoles in a condensed molecular system: The case of liquid water. <i>Physical Review B</i> , 2003 , 68,	3.3	33
82	Density-Polarization-Functional Theory and Long-Range Correlation in Dielectrics. <i>Physical Review Letters</i> , 1996 , 77, 2265-2267	7.4	33
81	Thermodynamic properties of Si-Ge alloys. <i>Physical Review B</i> , 1988 , 37, 6983-6990	3.3	33
80	Evidence of physical reality in the Kohn-Sham potential: The case of atomic Ne. <i>Physical Review A</i> , 1998 , 57, 2466-2469	2.6	32
79	Quantization of the dipole moment and of the end charges in push-pull polymers. <i>Journal of Chemical Physics</i> , 2007 , 127, 194902	3.9	30
78	Macroscopic polarization as a discrete Berry phase of the Hartree-Fock wave function: The single-point limit. <i>Physical Review B</i> , 1998 , 58, 1222-1229	3.3	30
77	Rydberg states in condensed matter. <i>Physical Review B</i> , 1979 , 19, 1683-1688	3.3	30
76	Dielectric matrices in semiconductors: A direct approach. <i>Physical Review B</i> , 1985 , 31, 5305-5310	3.3	28
75	Dielectric behavior of a doped semiconductor. <i>Physical Review B</i> , 1979 , 19, 3022-3026	3.3	28
74	Orbital magnetization as a local property. <i>Physical Review Letters</i> , 2013 , 110, 087202	7.4	27
73	Microscopic manipulation of homojunction band lineups. <i>Journal of Applied Physics</i> , 1992 , 71, 2048-2050	2.5	27
72	Local-field effects and phonon screening in polar semiconductors. <i>Physical Review B</i> , 1983 , 27, 3620-3630	3.3	27
71	Dielectric anomalies in ferroelectric nanostructures. <i>Physical Review Letters</i> , 2007 , 99, 227601	7.4	26
70	Orbital magnetization in extended systems. <i>ChemPhysChem</i> , 2005 , 6, 1815-9	3.2	26
69	Modern theory of polarization in ferroelectrics. <i>Ferroelectrics</i> , 1994 , 151, 49-58	0.6	26
68	Real-space equation for single-donor impurities and core excitons in many-valley semiconductors. <i>Physical Review B</i> , 1982 , 25, 4031-4037	3.3	25
67	Deformation-potential theorem in metals and in dielectrics. <i>Physical Review B</i> , 1991 , 44, 11035-11041	3.3	24

66	Local-field effects and zone-center phonons in Si, Ge, GaAs, and ZnSe. <i>Physical Review B</i> , 1981 , 24, 4839-4842	3.9	24
65	Berry phase approach to longitudinal dipole moments of infinite chains in electronic-structure methods with local basis sets. <i>Journal of Chemical Physics</i> , 2007 , 126, 234101	3.9	22
64	Macroscopic polarization from electronic wave functions. <i>International Journal of Quantum Chemistry</i> , 1999 , 75, 599-606	2.1	22
63	Core excitons in solid rare gases: Nonstructural theory. <i>Physical Review B</i> , 1978 , 18, 702-710	3.3	22
62	Longitudinal polarizability of long polymeric chains: quasi-one-dimensional electrostatics as the origin of slow convergence. <i>Journal of Chemical Physics</i> , 2005 , 122, 134907	3.9	21
61	Theory of band offsets at semiconductor heterojunctions: An ab-initio linear response approach. <i>Superlattices and Microstructures</i> , 1989 , 6, 31-37	2.8	21
60	Piezoelectricity in III-V and II-VI semiconductors: A systematic ab-initio calculation. <i>Ferroelectrics</i> , 1990 , 111, 19-22	0.6	20
59	A note on the many-valley effective mass theory. <i>Journal of Physics C: Solid State Physics</i> , 1977 , 10, L179-L182		20
58	Electron Band Structure of Solid Methane: Ab Initio Calculations. <i>Physical Review B</i> , 1973 , 7, 5321-5329	3.3	20
57	Can We Tune the Band Offset at Semiconductor Heterojunctions?. <i>NATO ASI Series Series B: Physics</i> , 1989 , 251-271		19
56	Effects of interface morphology on Schottky-barrier heights: A case study on Al/GaAs(001). <i>Physical Review B</i> , 1997 , 56, 14921-14924	3.3	18
55	Polarization fluctuations in insulators and metals: new and old theories merge. <i>Physical Review Letters</i> , 2006 , 96, 137601	7.4	18
54	Structural and electronic properties of strained Si/GaAs heterostructures. <i>Physical Review B</i> , 1993 , 48, 12047-12052	3.3	18
53	Kohn's localization in the insulating state: one-dimensional lattices, crystalline versus disordered. <i>Journal of Chemical Physics</i> , 2010 , 133, 064703	3.9	17
52	Surface reconstructions and bonding via the electron localization function: the case of Si(001). <i>Solid State Communications</i> , 1999 , 111, 583-588	1.6	17
51	Energy Bands in Cubic Ice. Ab Initio Calculation Using the Method of Linear Combination of Molecular Orbitals. <i>Physica Status Solidi (B): Basic Research</i> , 1977 , 81, 129-138	1.3	17
50	How disorder affects the Berry-phase anomalous Hall conductivity: A reciprocal-space analysis. <i>Physical Review B</i> , 2014 , 90,	3.3	16
49	Dynamical-charge neutrality at a crystal surface. <i>Physical Review B</i> , 1998 , 57, 5742-5745	3.3	16

48	Ionized impurity scattering in semiconductors. <i>Physical Review B</i> , 1979 , 20, 3254-3257	3.3	16
47	Isotropic Compton Profile of LiH in the Tight-Binding Approximation. <i>Physica Status Solidi (B): Basic Research</i> , 1976 , 73, 371-378	1.3	16
46	Quantum defect theory of excitons solid neon. <i>Physica Status Solidi (B): Basic Research</i> , 1978 , 86, 627-633.	3.3	16
45	Locality of the anomalous Hall conductivity. <i>Physical Review B</i> , 2017 , 95,	3.3	15
44	Single-donor impurities and core excitons in many-valley semiconductors. <i>Physical Review B</i> , 1982 , 25, 4038-4044	3.3	14
43	Spontaneous polarization from first-principles: Pyroelectric BeO. <i>Ferroelectrics</i> , 1990 , 111, 15-17	0.6	13
42	Study of correlation holes. II. CI calculations on model polyatomic systems. <i>International Journal of Quantum Chemistry</i> , 1981 , 19, 301-318	2.1	13
41	Hartree-Fock approach to macroscopic polarization: Dielectric constant and dynamical charges of KNbO ₃ . <i>Physical Review B</i> , 1998 , 57, 6967-6971	3.3	12
40	Baldereschi, Posternak, and Resta reply. <i>Physical Review Letters</i> , 1992 , 69, 390	7.4	12
39	Electron band structure of solid methane: Inclusion of intermolecular self-consistency in calculations. <i>Physical Review B</i> , 1974 , 9, 5332-5333	3.3	12
38	Drude weight and superconducting weight. <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 414001	1.8	12
37	Irrelevance of the Boundary on the Magnetization of Metals. <i>Physical Review Letters</i> , 2016 , 116, 137201	7.4	11
36	Orbital magnetization and Chern number in a supercell framework: Single k-point formula. <i>Physical Review B</i> , 2007 , 76,	3.3	11
35	Polarization properties of KNbO: comparison between Hartree-Fock and density-functional calculations. <i>Solid State Communications</i> , 1999 , 112, 465-470	1.6	10
34	Chapter 5 Quantum Electrostatics of Insulators: Polarization, Wannier Functions, and Electric Fields. <i>Contemporary Concepts of Condensed Matter Science</i> , 2006 , 2, 139-163		9
33	Bound state properties of H ₂ by the many-body green's function method. <i>Chemical Physics Letters</i> , 1976 , 37, 556-560	2.5	9
32	Role of covalence and of correlation in the dielectric polarization of oxides. <i>Ferroelectrics</i> , 1997 , 194, 1-9	0.6	8
31	Relationships between the semiempirical and the Hartree-Fock methods in band structure calculations. <i>Solid State Communications</i> , 1980 , 34, 461-465	1.6	8

30	The use of electron-atom scattering phase shifts in conduction-band calculations: Application to solid argon. <i>Journal of Physics C: Solid State Physics</i> , 1976 , 9, 2313-2317		8
29	Electronic excitations of the rare-gases in the solid phase. <i>Solid State Communications</i> , 1978 , 26, 849-851	1.6	8
28	Polarization in Kohn-Sham density-functional theory. <i>European Physical Journal B</i> , 2018 , 91, 1	1.2	7
27	Lyddane-Sachs-Teller relationship in linear magnetoelectrics. <i>Physical Review Letters</i> , 2011 , 106, 047202	7.4	7
26	Local Theory of the Insulating State. <i>Physical Review Letters</i> , 2019 , 122, 166602	7.4	6
25	Resta Replies:. <i>Physical Review Letters</i> , 1997 , 78, 2030-2030	7.4	6
24	The use of electron-atom scattering phase shifts in conduction band calculations. Solid neon. <i>Journal of Physics C: Solid State Physics</i> , 1977 , 10, L477-L479		6
23	Study of correlation holes. I. Number of rules and infinite system. <i>International Journal of Quantum Chemistry</i> , 1978 , 14, 171-179	2.1	6
22	Dynamical charges in oxides: recent advances. <i>Journal of Physics and Chemistry of Solids</i> , 2000 , 61, 153-157	3.9	5
21	Simple method for constructing accurate atomic Kohn-Sham potentials. <i>Physical Review A</i> , 1999 , 60, 3541-3546	3.5	5
20	Orbital magnetization in insulators: Bulk versus surface. <i>Physical Review B</i> , 2016 , 93,	3.3	4
19	Magnetic circular dichroism versus orbital magnetization. <i>Physical Review Research</i> , 2020 , 2,	3.9	4
18	Why are insulators insulating and metals conducting?. <i>Europhysics News</i> , 2003 , 34, 92-94	0.2	3
17	Neglecting local-field effects in the band-offset problem. <i>Journal of Physics Condensed Matter</i> , 1990 , 2, 10217-10222	1.8	3
16	Microscopic electronic screening in semiconductors 1985 , 183-194		3
15	Macroscopic Dielectric Polarization: Hartree-Fock Theory. <i>Lecture Notes in Quantum Chemistry II</i> , 1996 , 273-288	0.6	3
14	Metal-insulator transition in disordered systems from the one-body density matrix. <i>Physical Review B</i> , 2017 , 95,	3.3	2
13	N-representability and density-functional construction in curvilinear coordinates. <i>Solid State Communications</i> , 1998 , 106, 763-768	1.6	2

12	Macroscopic polarization in crystalline dielectrics. <i>Computational and Theoretical Chemistry</i> , 2004 , 709, 201-205		2
11	Quantum mechanism of polarization in perovskites. <i>Ferroelectrics</i> , 1995 , 164, 153-159	0.6	2
10	Bulk excitons in solid neon: Theory. <i>Physical Review B</i> , 1980 , 21, 4889-4891	3.3	2
9	Valence energy bands of solid hydrogen in H.C.P. structure. Ab initio LCMO calculation. <i>Physica Status Solidi (B): Basic Research</i> , 1975 , 69, 127-132	1.3	2
8	From the dipole of a crystallite to the polarization of a crystal. <i>Journal of Chemical Physics</i> , 2021 , 154, 050901	3.9	2
7	Drude weight in systems with open boundary conditions. <i>Physical Review B</i> , 2020 , 102,	3.3	1
6	Screening of a point charge in semiconductors and insulators. <i>Physical Review B</i> , 1988 , 38, 818	3.3	1
5	Ionized impurity scattering in semimetals. <i>Physical Review B</i> , 1980 , 22, 3935-3938	3.3	1
4	Faraday law, oxidation numbers, and ionic conductivity: The role of topology.. <i>Journal of Chemical Physics</i> , 2021 , 155, 244503	3.9	0
3	Dielectric Polarization of Materials: A Modern View. <i>Materials Research Society Symposia Proceedings</i> , 2001 , 677, 611		
2	Electrical Polarization and Orbital Magnetization: The Position Operator Tamed 2020 , 151-181		
1	Electrical Polarization and Orbital Magnetization: The Position Operator Tamed 2018 , 1-31		