Raffaele Resta

List of Publications by Year in Descending Order

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	Faraday law, oxidation numbers, and ionic conductivity: The role of topology.. *Journal of Chemical Physics*, **2021**, 155, 244503	3.9	0
136	From the dipole of a crystallite to the polarization of a crystal. *Journal of Chemical Physics*, **2021**, 154, 050901	3.9	2
135	Drude weight in systems with open boundary conditions. *Physical Review B*, **2020**, 102,	3.3	1
134	Magnetic circular dichroism versus orbital magnetization. *Physical Review Research*, **2020**, 2,	3.9	4
133	Electrical Polarization and Orbital Magnetization: The Position Operator Tamed **2020**, 151-181		
132	Local Theory of the Insulating State. *Physical Review Letters*, **2019**, 122, 166602	7.4	6
131	Polarization in Kohn-Sham density-functional theory. *European Physical Journal B*, **2018**, 91, 1	1.2	7
130	Electrical Polarization and Orbital Magnetization: The Position Operator Tamed **2018**, 1-31		
129	Drude weight and superconducting weight. *Journal of Physics Condensed Matter*, **2018**, 30, 414001	1.8	12
128	Metal-insulator transition in disordered systems from the one-body density matrix. *Physical Review B*, **2017**, 95,	3.3	2
127	Locality of the anomalous Hall conductivity. *Physical Review B*, **2017**, 95,	3.3	15
126	Orbital magnetization in insulators: Bulk versus surface. *Physical Review B*, **2016**, 93,	3.3	4
125	Irrelevance of the Boundary on the Magnetization of Metals. *Physical Review Letters*, **2016**, 116, 137201	7.4	11
124	How disorder affects the Berry-phase anomalous Hall conductivity: A reciprocal-space analysis. *Physical Review B*, **2014**, 90,	3.3	16
123	Orbital magnetization as a local property. *Physical Review Letters*, **2013**, 110, 087202	7.4	27
122	Lyddane-Sachs-Teller relationship in linear magnetoelectrics. *Physical Review Letters*, **2011**, 106, 047202	7.4	7
121	Mapping topological order in coordinate space. *Physical Review B*, **2011**, 84,	3.3	79

120	The insulating state of matter: a geometrical theory. *European Physical Journal B*, **2011**, 79, 121-137	1.2	112
119	Towards a bulk theory of flexoelectricity. *Physical Review Letters*, **2010**, 105, 127601	7.4	109
118	Kohn's localization in the insulating state: one-dimensional lattices, crystalline versus disordered. *Journal of Chemical Physics*, **2010**, 133, 064703	3.9	17
117	Electrical polarization and orbital magnetization: the modern theories. *Journal of Physics Condensed Matter*, **2010**, 22, 123201	1.8	106
116	A converse approach to the calculation of NMR shielding tensors. *Journal of Chemical Physics*, **2009**, 131, 101101	3.9	49
115	Role of dipolar correlations in the infrared spectra of water and ice. *Physical Review B*, **2008**, 77,	3.3	59
114	Theory of Polarization: A Modern Approach **2007**, 31-68		176
113	Dipolar correlations and the dielectric permittivity of water. *Physical Review Letters*, **2007**, 98, 247401	7.4	138
112	Berry phase approach to longitudinal dipole moments of infinite chains in electronic-structure methods with local basis sets. *Journal of Chemical Physics*, **2007**, 126, 234101	3.9	22
111	Quantization of the dipole moment and of the end charges in push-pull polymers. *Journal of Chemical Physics*, **2007**, 127, 194902	3.9	30
110	Dielectric anomalies in ferroelectric nanostructures. *Physical Review Letters*, **2007**, 99, 227601	7.4	26
109	Orbital magnetization and Chern number in a supercell framework: Single k-point formula. *Physical Review B*, **2007**, 76,	3.3	11
108	Polarization fluctuations in insulators and metals: new and old theories merge. *Physical Review Letters*, **2006**, 96, 137601	7.4	18
107	Kohn's theory of the insulating state: a quantum-chemistry viewpoint. *Journal of Chemical Physics*, **2006**, 124, 104104	3.9	53
106	Chapter 5 Quantum Electrostatics of Insulators: Polarization, Wannier Functions, and Electric Fields. *Contemporary Concepts of Condensed Matter Science*, **2006**, 2, 139-163		9
105	Intermolecular dynamical charge fluctuations in water: a signature of the H-bond network. *Physical Review Letters*, **2005**, 95, 187401	7.4	121
104	Orbital magnetization in periodic insulators. *Physical Review Letters*, **2005**, 95, 137205	7.4	227
103	Orbital magnetization in extended systems. *ChemPhysChem*, **2005**, 6, 1815-9	3.2	26

102	Longitudinal polarizability of long polymeric chains: quasi-one-dimensional electrostatics as the origin of slow convergence. *Journal of Chemical Physics*, **2005**, 122, 134907	3.9	21
101	Electron localization in the quantum Hall regime. *Physical Review Letters*, **2005**, 95, 196805	7.4	35
100	Macroscopic polarization in crystalline dielectrics. *Computational and Theoretical Chemistry*, **2004**, 709, 201-205		2
99	Why are insulators insulating and metals conducting?. *Europhysics News*, **2003**, 34, 92-94	0.2	3
98	Ab initio simulation of the properties of ferroelectric materials. *Modelling and Simulation in Materials Science and Engineering*, **2003**, 11, R69-R96	2	44
97	Dynamical monopoles and dipoles in a condensed molecular system: The case of liquid water. *Physical Review B*, **2003**, 68,	3.3	33
96	Why are insulators insulating and metals conducting?. *Journal of Physics Condensed Matter*, **2002**, 14, R625-R656	1.8	142
95	Electron localization in the insulating state: Application to crystalline semiconductors. *Physical Review B*, **2001**, 64,	3.3	106
94	Dielectric Polarization of Materials: A Modern View. *Materials Research Society Symposia Proceedings*, **2001**, 677, 611		
93	Dynamical charges in oxides: recent advances. *Journal of Physics and Chemistry of Solids*, **2000**, 61, 153-157	3.9	5
92	Electron localization at metal surfaces. *Surface Science*, **2000**, 450, 126-132	1.8	48
91	Manifestations of Berry's phase in molecules and condensed matter. *Journal of Physics Condensed Matter*, **2000**, 12, R107-R143	1.8	177
90	Electron Localization in the Insulating State. *Physical Review Letters*, **1999**, 82, 370-373	7.4	315
89	Hartree-Fock studies of surface properties of BaTiO3. *Physical Review B*, **1999**, 60, 2697-2703	3.3	57
88	Noncubic Behavior of Antiferromagnetic Transition-Metal Monoxides with the Rocksalt Structure. *Physical Review Letters*, **1999**, 82, 430-433	7.4	81
87	Simple method for constructing accurate atomic Kohn-Sham potentials. *Physical Review A*, **1999**, 60, 3541-3546	1.6	5
86	Surface reconstructions and bonding via the electron localization function: the case of Si(001). *Solid State Communications*, **1999**, 111, 583-588	1.6	17
85	Polarization properties of KNbO: comparison between Hartree-Fock and density-functional calculations. *Solid State Communications*, **1999**, 112, 465-470	1.6	10

84	Macroscopic polarization from electronic wave functions. *International Journal of Quantum Chemistry*, **1999**, 75, 599-606	2.1	22
83	N-representability and density-functional construction in curvilinear coordinates. *Solid State Communications*, **1998**, 106, 763-768	1.6	2
82	Quantum-Mechanical Position Operator in Extended Systems. *Physical Review Letters*, **1998**, 80, 1800-1803	7.4	420
81	Evidence of physical reality in the Kohn-Sham potential: The case of atomic Ne. *Physical Review A*, **1998**, 57, 2466-2469	2.6	32
80	Macroscopic polarization as a discrete Berry phase of the Hartree-Fock wave function: The single-point limit. *Physical Review B*, **1998**, 58, 1222-1229	3.3	30
79	Dynamical-charge neutrality at a crystal surface. *Physical Review B*, **1998**, 57, 5742-5745	3.3	16
78	Hartree-Fock approach to macroscopic polarization: Dielectric constant and dynamical charges of KNbO3. *Physical Review B*, **1998**, 57, 6967-6971	3.3	12
77	Resta Replies:. *Physical Review Letters*, **1997**, 78, 2030-2030	7.4	6
76	Effects of interface morphology on Schottky-barrier heights: A case study on Al/GaAs(001). *Physical Review B*, **1997**, 56, 14921-14924	3.3	18
75	Spontaneous polarization as a Berry phase of the Hartree-Fock wave function: The case of KNbO3. *Physical Review B*, **1997**, 56, 10105-10114	3.3	130
74	Role of covalence and of correlation in the dielectric polarization of oxides. *Ferroelectrics*, **1997**, 194, 1-9	0.6	8
73	Density-Polarization-Functional Theory and Long-Range Correlation in Dielectrics. *Physical Review Letters*, **1996**, 77, 2265-2267	7.4	33
72	Macroscopic Dielectric Polarization: Hartree-Fock Theory. *Lecture Notes in Quantum Chemistry II*, **1996**, 273-288	0.6	3
71	Quantum mechanism of polarization in perovskites. *Ferroelectrics*, **1995**, 164, 153-159	0.6	2
70	Many-body effects on polarization and dynamical charges in a partly covalent polar insulator. *Physical Review Letters*, **1995**, 74, 4738-4741	7.4	81
69	Modern theory of polarization in ferroelectrics. *Ferroelectrics*, **1994**, 151, 49-58	0.6	26
68	Density-functional theory of the dielectric constant: Gradient-corrected calculation for silicon. *Physical Review B*, **1994**, 49, 5323-5328	3.3	81
67	Role of covalent bonding in the polarization of perovskite oxides: The case of KNbO3. *Physical Review B*, **1994**, 50, 8911-8914	3.3	155

66	Density-functional theory of macroscopic stress: Gradient-corrected calculations for crystalline Se. *Physical Review B*, **1994**, 50, 4327-4331	3.3	61
65	Ab initio study of piezoelectricity and spontaneous polarization in ZnO. *Physical Review B*, **1994**, 50, 10715-10721	3.3	265
64	Macroscopic polarization in crystalline dielectrics: the geometric phase approach. *Reviews of Modern Physics*, **1994**, 66, 899-915	40.5	1651
63	Local interface composition and band discontinuities in heterovalent heterostructures. *Physical Review Letters*, **1994**, 72, 294-297	7.4	122
62	Nonlinear piezoelectricity in CdTe. *Physical Review B*, **1993**, 47, 16252-16256	3.3	41
61	Towards a quantum theory of polarization in ferroelectrics: The case of KNbO3. *Physical Review Letters*, **1993**, 70, 1010-1013	7.4	269
60	Structural and electronic properties of strained Si/GaAs heterostructures. *Physical Review B*, **1993**, 48, 12047-12052	3.3	18
59	Ab initio calculation of phonon dispersions in II-VI semiconductors. *Physical Review B*, **1993**, 47, 3588-3593	3.3	196
58	Macroscopic Electric Polarization as a Geometric Quantum Phase. *Europhysics Letters*, **1993**, 22, 133-138	1.6	139
57	Microscopic capacitors and neutral interfaces in III-V/IV/III-V semiconductor heterostructures. *Physical Review Letters*, **1992**, 69, 1283-1286	7.4	48
56	Microscopic manipulation of homojunction band lineups. *Journal of Applied Physics*, **1992**, 71, 2048-2050	2.5	27
55	Baldereschi, Posternak, and Resta reply. *Physical Review Letters*, **1992**, 69, 390	7.4	12
54	Theory of the electric polarization in crystals. *Ferroelectrics*, **1992**, 136, 51-55	0.6	319
53	Tuning band offsets at semiconductor interfaces by intralayer deposition. *Physical Review B*, **1991**, 43, 7347-7350	3.3	98
52	Deformation-potential theorem in metals and in dielectrics. *Physical Review B*, **1991**, 44, 11035-11041	3.3	24
51	Valence-band offsets at strained Si/Ge interfaces. *Physical Review B*, **1991**, 44, 5572-5579	3.3	168
50	Neglecting local-field effects in the band-offset problem. *Journal of Physics Condensed Matter*, **1990**, 2, 10217-10222	1.8	3
49	Ab initio study of the spontaneous polarization of pyroelectric BeO. *Physical Review Letters*, **1990**, 64, 1777-1780	7.4	101

48	Electronic structure of InP/Ga0.47In0.53As interfaces. *Physical Review B*, **1990**, 41, 12106-12110	3.3	38
47	Piezoelectricity in III-V and II-VI semiconductors: A systematic ab-initio calculation. *Ferroelectrics*, **1990**, 111, 19-22	0.6	20
46	Spontaneous polarization from first-principles: Pyroelectric BeO. *Ferroelectrics*, **1990**, 111, 15-17	0.6	13
45	Absolute deformation potentials in semiconductors. *Physical Review B*, **1990**, 41, 12358-12361	3.3	46
44	Theory of band offsets at semiconductor heterojunctions: An ab-initio linear response approach. *Superlattices and Microstructures*, **1989**, 6, 31-37	2.8	21
43	Piezoelectric properties of III-V semiconductors from first-principles linear-response theory. *Physical Review Letters*, **1989**, 62, 2853-2856	7.4	161
42	Can We Tune the Band Offset at Semiconductor Heterojunctions?. *NATO ASI Series Series B: Physics*, **1989**, 251-271		19
41	Microscopic atomic structure and stability of Si-Ge solid solutions. *Physical Review B*, **1988**, 37, 1308-1314	3.3	53
40	Band offsets in lattice-matched heterojunctions: A model and first-principles calculations for GaAs/AlAs. *Physical Review Letters*, **1988**, 61, 734-737	7.4	465
39	Thermodynamic properties of Si-Ge alloys. *Physical Review B*, **1988**, 37, 6983-6990	3.3	33
38	Screening of a point charge in semiconductors and insulators. *Physical Review B*, **1988**, 38, 818	3.3	1
37	Real-space force constants for lattice dynamics in silicon and germanium in the adiabatic bond-charge model. *Physical Review B*, **1986**, 34, 7140-7145	3.3	47
36	Ab initio calculation of the low-frequency Raman cross section in silicon. *Physical Review B*, **1986**, 33, 5969-5971	3.3	55
35	Self-consistent theory of electronic states and dielectric response in semiconductors. *Physical Review B*, **1986**, 34, 7146-7157	3.3	125
34	Ab initio calculation of the macroscopic dielectric constant in silicon. *Physical Review B*, **1986**, 33, 7017-7021	3.3	406
33	Microscopic electronic screening in semiconductors **1985**, 183-194		3
32	Dielectric matrices in semiconductors: A direct approach. *Physical Review B*, **1985**, 31, 5305-5310	3.3	28
31	External Fields in the Self-Consistent Theory of Electronic States: A New Method for Direct Evaluation of Macroscopic and Microscopic Dielectric Response. *Physical Review Letters*, **1983**, 51, 686-689	7.4	90

30	Local-field effects and phonon screening in polar semiconductors. *Physical Review B*, **1983**, 27, 3620-3630	3.3	27
29	Single-donor impurities and core excitons in many-valley semiconductors. *Physical Review B*, **1982**, 25, 4038-4044	3.3	14
28	Real-space equation for single-donor impurities and core excitons in many-valley semiconductors. *Physical Review B*, **1982**, 25, 4031-4037	3.3	25
27	Local-field effects and zone-center phonons in Si, Ge, GaAs, and ZnSe. *Physical Review B*, **1981**, 24, 4839-4842	3.3	24
26	Study of correlation holes. II. CI calculations on model polyatomic systems. *International Journal of Quantum Chemistry*, **1981**, 19, 301-318	2.1	13
25	Dielectric matrices and local fields in polar semiconductors. *Physical Review B*, **1981**, 23, 6615-6624	3.3	54
24	Relationships between the semiempirical and the Hartree-Fock methods in band structure calculations. *Solid State Communications*, **1980**, 34, 461-465	1.6	8
23	Bulk excitons in solid neon: Theory. *Physical Review B*, **1980**, 21, 4889-4891	3.3	2
22	Ionized impurity scattering in semimetals. *Physical Review B*, **1980**, 22, 3935-3938	3.3	1
21	Shallow-Deep Instabilities of Donor Impurity Levels and Excitons in Many-Valley Semiconductors. *Physical Review Letters*, **1980**, 44, 1340-1344	7.4	63
20	Large binding due to dispersive screening and bloch function interference in many-valley semiconductors. *Solid State Communications*, **1979**, 29, 275-277	1.6	47
19	Ionized impurity scattering in semiconductors. *Physical Review B*, **1979**, 20, 3254-3257	3.3	16
18	Rydberg states in condensed matter. *Physical Review B*, **1979**, 19, 1683-1688	3.3	30
17	Dielectric behavior of a doped semiconductor. *Physical Review B*, **1979**, 19, 3022-3026	3.3	28
16	Study of correlation holes. I. Number sum rules and infinite system. *International Journal of Quantum Chemistry*, **1978**, 14, 171-179	2.1	6
15	Quantum defect theory of excitons solid neon. *Physica Status Solidi (B): Basic Research*, **1978**, 86, 627-633	1.3	16
14	Electronic excitations of the rare-gases in the solid phase. *Solid State Communications*, **1978**, 26, 849-851	1.6	8
13	Nonlinear impurity screening in semiconductors. *Physical Review B*, **1978**, 17, 3239-3242	3.3	64

12	Nonstructural theory of the exciton states in solid rare gases. *Physical Review B*, **1978**, 18, 696-701	3.3	45
11	Core excitons in solid rare gases: Nonstructural theory. *Physical Review B*, **1978**, 18, 702-710	3.3	22
10	The use of electron-atom scattering phase shifts in conduction band calculations. Solid neon. *Journal of Physics C: Solid State Physics*, **1977**, 10, L477-L479		6
9	A note on the many-valley effective mass theory. *Journal of Physics C: Solid State Physics*, **1977**, 10, L179-L182		20
8	Thomas-Fermi dielectric screening in semiconductors. *Physical Review B*, **1977**, 16, 2717-2722	3.3	231
7	Energy Bands in Cubic Ice. Ab Initio Calculation Using the Method of Linear Combination of Molecular Orbitals. *Physica Status Solidi (B): Basic Research*, **1977**, 81, 129-138	1.3	17
6	Isotropic Compton Profile of LiH in the Tight-Binding Approximation. *Physica Status Solidi (B): Basic Research*, **1976**, 73, 371-378	1.3	16
5	Bound state properties of H2 by the many-body green's function method. *Chemical Physics Letters*, **1976**, 37, 556-560	2.5	9
4	The use of electron-atom scattering phase shifts in conduction-band calculations: Application to solid argon. *Journal of Physics C: Solid State Physics*, **1976**, 9, 2313-2317		8
3	Valence energy bands of solid hydrogen in H.C.P. structure. Ab initio LCMO calculation. *Physica Status Solidi (B): Basic Research*, **1975**, 69, 127-132	1.3	2
2	Electron band structure of solid methane: Inclusion of intermolecular self-consistency in calculations. *Physical Review B*, **1974**, 9, 5332-5333	3.3	12
1	Electron Band Structure of Solid Methane: Ab Initio Calculations. *Physical Review B*, **1973**, 7, 5321-5329	3.3	20