

Raffaele Resta

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/5248597/publications.pdf>

Version: 2024-02-01

143
papers

11,776
citations

43973

48
h-index

28224

105
g-index

145
all docs

145
docs citations

145
times ranked

7318
citing authors

#	ARTICLE	IF	CITATIONS
1	Macroscopic polarization in crystalline dielectrics: the geometric phase approach. <i>Reviews of Modern Physics</i> , 1994, 66, 899-915.	16.4	2,016
2	Quantum-Mechanical Position Operator in Extended Systems. <i>Physical Review Letters</i> , 1998, 80, 1800-1803.	2.9	559
3	Band Offsets in Lattice-Matched Heterojunctions: A Model and First-Principles Calculations for GaAs/AlAs. <i>Physical Review Letters</i> , 1988, 61, 734-737.	2.9	507
4	Ab initio calculation of the macroscopic dielectric constant in silicon. <i>Physical Review B</i> , 1986, 33, 7017-7021.	1.1	499
5	Theory of the electric polarization in crystals. <i>Ferroelectrics</i> , 1992, 136, 51-55.	0.3	422
6	Electron Localization in the Insulating State. <i>Physical Review Letters</i> , 1999, 82, 370-373.	2.9	388
7	Towards a quantum theory of polarization in ferroelectrics: The case of KNbO ₃ . <i>Physical Review Letters</i> , 1993, 70, 1010-1013.	2.9	328
8	Ab initio study of piezoelectricity and spontaneous polarization in ZnO. <i>Physical Review B</i> , 1994, 50, 10715-10721.	1.1	305
9	Orbital Magnetization in Periodic Insulators. <i>Physical Review Letters</i> , 2005, 95, 137205.	2.9	300
10	Thomas-Fermi dielectric screening in semiconductors. <i>Physical Review B</i> , 1977, 16, 2717-2722.	1.1	254
11	Theory of Polarization: A Modern Approach. , 2007, , 31-68.		231
12	Ab initio calculation of phonon dispersions in II-VI semiconductors. <i>Physical Review B</i> , 1993, 47, 3588-3592.	1.1	229
13	Manifestations of Berry's phase in molecules and condensed matter. <i>Journal of Physics Condensed Matter</i> , 2000, 12, R107-R143.	0.7	229
14	Piezoelectric properties of III-V semiconductors from first-principles linear-response theory. <i>Physical Review Letters</i> , 1989, 62, 2853-2856.	2.9	221
15	Why are insulators insulating and metals conducting?. <i>Journal of Physics Condensed Matter</i> , 2002, 14, R625-R656.	0.7	185
16	Macroscopic Electric Polarization as a Geometric Quantum Phase. <i>Europhysics Letters</i> , 1993, 22, 133-138.	0.7	183
17	Valence-band offsets at strained Si/Ge interfaces. <i>Physical Review B</i> , 1991, 44, 5572-5579.	1.1	177
18	Role of covalent bonding in the polarization of perovskite oxides: The case of KNbO ₃ . <i>Physical Review B</i> , 1994, 50, 8911-8914.	1.1	166

#	ARTICLE	IF	CITATIONS
19	The insulating state of matter: a geometrical theory. <i>European Physical Journal B</i> , 2011, 79, 121-137.	0.6	164
20	Mapping topological order in coordinate space. <i>Physical Review B</i> , 2011, 84, .	1.1	155
21	Dipolar Correlations and the Dielectric Permittivity of Water. <i>Physical Review Letters</i> , 2007, 98, 247401.	2.9	153
22	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.	1.1	151
23	Self-consistent theory of electronic states and dielectric response in semiconductors. <i>Physical Review B</i> , 1986, 34, 7146-7157.	1.1	150
24	Towards a Bulk Theory of Flexoelectricity. <i>Physical Review Letters</i> , 2010, 105, 127601.	2.9	140
25	Electron localization in the insulating state: Application to crystalline semiconductors. <i>Physical Review B</i> , 2001, 64, .	1.1	136
26	Electrical polarization and orbital magnetization: the modern theories. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 123201.	0.7	134
27	Intermolecular Dynamical Charge Fluctuations in Water: A Signature of the H-Bond Network. <i>Physical Review Letters</i> , 2005, 95, 187401.	2.9	133
28	Local interface composition and band discontinuities in heterovalent heterostructures. <i>Physical Review Letters</i> , 1994, 72, 294-297.	2.9	130
29	Ab initio study of the spontaneous polarization of pyroelectric BeO. <i>Physical Review Letters</i> , 1990, 64, 1777-1780.	2.9	108
30	Tuning band offsets at semiconductor interfaces by intralayer deposition. <i>Physical Review B</i> , 1991, 43, 7347-7350.	1.1	103
31	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.	2.9	99
32	Noncubic Behavior of Antiferromagnetic Transition-Metal Monoxides with the Rocksalt Structure. <i>Physical Review Letters</i> , 1999, 82, 430-433.	2.9	91
33	Many-Body Effects on Polarization and Dynamical Charges in a Partly Covalent Polar Insulator. <i>Physical Review Letters</i> , 1995, 74, 4738-4741.	2.9	90
34	Density-functional theory of the dielectric constant: Gradient-corrected calculation for silicon. <i>Physical Review B</i> , 1994, 49, 5323-5328.	1.1	87
35	Ab initio calculation of the low-frequency Raman cross section in silicon. <i>Physical Review B</i> , 1986, 33, 5969-5971.	1.1	67
36	Density-functional theory of macroscopic stress: Gradient-corrected calculations for crystalline Se. <i>Physical Review B</i> , 1994, 50, 4327-4331.	1.1	67

#	ARTICLE	IF	CITATIONS
37	Kohn's theory of the insulating state: A quantum-chemistry viewpoint. <i>Journal of Chemical Physics</i> , 2006, 124, 104104.	1.2	67
38	Role of dipolar correlations in the infrared spectra of water and ice. <i>Physical Review B</i> , 2008, 77, .	1.1	67
39	Shallow-Deep Instabilities of Donor Impurity Levels and Excitons in Many-Valley Semiconductors. <i>Physical Review Letters</i> , 1980, 44, 1340-1344.	2.9	66
40	Nonlinear impurity screening in semiconductors. <i>Physical Review B</i> , 1978, 17, 3239-3242.	1.1	64
41	Hartree-Fock studies of surface properties of BaTiO ₃ . <i>Physical Review B</i> , 1999, 60, 2697-2703.	1.1	62
42	Dielectric matrices and local fields in polar semiconductors. <i>Physical Review B</i> , 1981, 23, 6615-6624.	1.1	61
43	Electron localization at metal surfaces. <i>Surface Science</i> , 2000, 450, 126-132.	0.8	59
44	Microscopic atomic structure and stability of Si-Ge solid solutions. <i>Physical Review B</i> , 1988, 37, 1308-1314.	1.1	57
45	Piezoelectricity in III-V and II-VI semiconductors: A systematic ab-initio calculation. <i>Ferroelectrics</i> , 1990, 111, 19-22.	0.3	55
46	A converse approach to the calculation of NMR shielding tensors. <i>Journal of Chemical Physics</i> , 2009, 131, 101101.	1.2	54
47	Microscopic capacitors and neutral interfaces in III-V/IV/III-V semiconductor heterostructures. <i>Physical Review Letters</i> , 1992, 69, 1283-1286.	2.9	52
48	Large binding due to dispersive screening and Bloch function interference in many-valley semiconductors. <i>Solid State Communications</i> , 1979, 29, 275-277.	0.9	50
49	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.	1.1	49
50	Absolute deformation potentials in semiconductors. <i>Physical Review B</i> , 1990, 41, 12358-12361.	1.1	49
51	Charge states in transition. <i>Nature</i> , 2008, 453, 735-735.	13.7	49
52	Nonlinear piezoelectricity in CdTe. <i>Physical Review B</i> , 1993, 47, 16252-16256.	1.1	48
53	Orbital Magnetization as a Local Property. <i>Physical Review Letters</i> , 2013, 110, 087202.	2.9	48
54	Ab initio simulation of the properties of ferroelectric materials. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2003, 11, R69-R96.	0.8	46

#	ARTICLE	IF	CITATIONS
55	Nonstructural theory of the exciton states in solid rare gases. <i>Physical Review B</i> , 1978, 18, 696-701.	1.1	45
56	Electronic structure of InP/Ga _{0.47} In _{0.53} As interfaces. <i>Physical Review B</i> , 1990, 41, 12106-12110.	1.1	40
57	Electron Localization in the Quantum Hall Regime. <i>Physical Review Letters</i> , 2005, 95, 196805.	2.9	39
58	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.	1.1	36
59	Thermodynamic properties of Si-Ge alloys. <i>Physical Review B</i> , 1988, 37, 6983-6990.	1.1	35
60	Modern theory of polarization in ferroelectrics. <i>Ferroelectrics</i> , 1994, 151, 49-58.	0.3	34
61	Density-Polarization-Functional Theory and Long-Range Correlation in Dielectrics. <i>Physical Review Letters</i> , 1996, 77, 2265-2267.	2.9	34
62	Dynamical monopoles and dipoles in a condensed molecular system: The case of liquid water. <i>Physical Review B</i> , 2003, 68, .	1.1	34
63	Quantization of the dipole moment and of the end charges in push-pull polymers. <i>Journal of Chemical Physics</i> , 2007, 127, 194902.	1.2	34
64	Local-field effects and zone-center phonons in Si, Ge, GaAs, and ZnSe. <i>Physical Review B</i> , 1981, 24, 4839-4842.	1.1	33
65	Evidence of physical reality in the Kohn-Sham potential: The case of atomic Ne. <i>Physical Review A</i> , 1998, 57, 2466-2469.	1.0	33
66	Dielectric Anomalies in Ferroelectric Nanostructures. <i>Physical Review Letters</i> , 2007, 99, 227601.	2.9	32
67	Rydberg states in condensed matter. <i>Physical Review B</i> , 1979, 19, 1683-1688.	1.1	31
68	Dielectric behavior of a doped semiconductor. <i>Physical Review B</i> , 1979, 19, 3022-3026.	1.1	30
69	Local-field effects and phonon screening in polar semiconductors. <i>Physical Review B</i> , 1983, 27, 3620-3630.	1.1	30
70	Dielectric matrices in semiconductors: A direct approach. <i>Physical Review B</i> , 1985, 31, 5305-5310.	1.1	30
71	Microscopic manipulation of homojunction band lineups. <i>Journal of Applied Physics</i> , 1992, 71, 2048-2050.	1.1	30
72	Locality of the anomalous Hall conductivity. <i>Physical Review B</i> , 2017, 95, .	1.1	30

#	ARTICLE	IF	CITATIONS
73	Orbital Magnetization in Extended Systems. ChemPhysChem, 2005, 6, 1815-1819.	1.0	28
74	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.	1.2	27
75	Deformation-potential theorem in metals and in dielectrics. Physical Review B, 1991, 44, 11035-11041.	1.1	26
76	Real-space equation for single-donor impurities and core excitons in many-valley semiconductors. Physical Review B, 1982, 25, 4031-4037.	1.1	25
77	Drude weight and superconducting weight. Journal of Physics Condensed Matter, 2018, 30, 414001.	0.7	24
78	Electron Band Structure of Solid Methane: Ab Initio Calculations. Physical Review B, 1973, 7, 5321-5329.	1.1	23
79	Kohn's localization in the insulating state: One-dimensional lattices, crystalline versus disordered. Journal of Chemical Physics, 2010, 133, 064703.	1.2	23
80	Core excitons in solid rare gases: Nonstructural theory. Physical Review B, 1978, 18, 702-710.	1.1	22
81	Theory of band offsets at semiconductor heterojunctions: An ab-initio linear response approach. Superlattices and Microstructures, 1989, 6, 31-37.	1.4	22
82	Macroscopic polarization from electronic wave functions. International Journal of Quantum Chemistry, 1999, 75, 599-606.	1.0	22
83	A note on the many-valley effective mass theory. Journal of Physics C: Solid State Physics, 1977, 10, L179-L182.	1.5	21
84	Surface reconstructions and bonding via the electron localization function: the case of Si(001). Solid State Communications, 1999, 111, 583-588.	0.9	21
85	Longitudinal polarizability of long polymeric chains: Quasi-one-dimensional electrostatics as the origin of slow convergence. Journal of Chemical Physics, 2005, 122, 134907.	1.2	21
86	How disorder affects the Berry-phase anomalous Hall conductivity: A reciprocal-space analysis. Physical Review B, 2014, 90, .	1.1	21
87	Can We Tune the Band Offset at Semiconductor Heterojunctions?. NATO ASI Series Series B: Physics, 1989, , 251-271.	0.2	21
88	Orbital magnetization and Chern number in a supercell framework: Single \mathbf{k} -point formula. Physical Review B, 2007, 76, .	1.1	20
89	Structural and electronic properties of strained Si/GaAs heterostructures. Physical Review B, 1993, 48, 12047-12052.	1.1	19
90	Effects of interface morphology on Schottky-barrier heights: A case study on Al/GaAs(001). Physical Review B, 1997, 56, 14921-14924.	1.1	19

#	ARTICLE	IF	CITATIONS
91	Polarization Fluctuations in Insulators and Metals: New and Old Theories Merge. Physical Review Letters, 2006, 96, 137601.	2.9	19
92	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.	0.7	18
93	Isotropic Compton Profile of LiH in the Tight-Binding Approximation. Physica Status Solidi (B): Basic Research, 1976, 73, 371-378.	0.7	16
94	Quantum defect theory of excitons solid neon. Physica Status Solidi (B): Basic Research, 1978, 86, 627-633.	0.7	16
95	Ionized impurity scattering in semiconductors. Physical Review B, 1979, 20, 3254-3257.	1.1	16
96	Dynamical-charge neutrality at a crystal surface. Physical Review B, 1998, 57, 5742-5745.	1.1	16
97	Irrelevance of the Boundary on the Magnetization of Metals. Physical Review Letters, 2016, 116, 137201.	2.9	16
98	Single-donor impurities and core excitons in many-valley semiconductors. Physical Review B, 1982, 25, 4038-4044.	1.1	14
99	Spontaneous polarization from first-principles: Pyroelectric BeO. Ferroelectrics, 1990, 111, 15-17.	0.3	14
100	Hartree-Fock approach to macroscopic polarization: Dielectric constant and dynamical charges of KNbO ₃ . Physical Review B, 1998, 57, 6967-6971.	1.1	14
101	Study of correlation holes. II. CI calculations on model polyatomic systems. International Journal of Quantum Chemistry, 1981, 19, 301-318.	1.0	13
102	Baldereschi, Posternak, and Resta reply. Physical Review Letters, 1992, 69, 390-390.	2.9	13
103	Electron band structure of solid methane: Inclusion of intermolecular self-consistency in calculations. Physical Review B, 1974, 9, 5332-5333.	1.1	12
104	Polarization properties of KNbO ₃ : comparison between Hartree-Fock and density-functional calculations. Solid State Communications, 1999, 112, 465-470.	0.9	12
105	Chapter 5 Quantum Electrostatics of Insulators: Polarization, Wannier Functions, and Electric Fields. Contemporary Concepts of Condensed Matter Science, 2006, 2, 139-163.	0.5	12
106	Local Theory of the Insulating State. Physical Review Letters, 2019, 122, 166602.	2.9	11
107	Bound state properties of H ₂ by the many-body green's function method. Chemical Physics Letters, 1976, 37, 556-560.	1.2	10
108	Orbital magnetization in insulators: Bulk versus surface. Physical Review B, 2016, 93, .	1.1	10

#	ARTICLE	IF	CITATIONS
109	Polarization in Kohn-Sham density-functional theory. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	10
110	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.	1.5	8
111	Electronic excitations of the rare-gases in the solid phase. <i>Solid State Communications</i> , 1978, 26, 849-851.	0.9	8
112	Relationships between the semiempirical and the Hartree-Fock methods in band structure calculations. <i>Solid State Communications</i> , 1980, 34, 461-465.	0.9	8
113	Role of covalence and of correlation in the dielectric polarization of oxides. <i>Ferroelectrics</i> , 1997, 194, 1-9.	0.3	8
114	Lyddane-Sachs-Teller Relationship in Linear Magnetoelectrics. <i>Physical Review Letters</i> , 2011, 106, 047202.	2.9	8
115	Resta Replies:. <i>Physical Review Letters</i> , 1997, 78, 2030-2030.	2.9	7
116	Magnetic circular dichroism versus orbital magnetization. <i>Physical Review Research</i> , 2020, 2, .	1.3	7
117	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.	1.5	6
118	Study of correlation holes. I. Number-sum rules and infinite system. <i>International Journal of Quantum Chemistry</i> , 1978, 14, 171-179.	1.0	6
119	Simple method for constructing accurate atomic Kohn-Sham potentials. <i>Physical Review A</i> , 1999, 60, 3541-3546.	1.0	6
120	Dynamical charges in oxides: recent advances. <i>Journal of Physics and Chemistry of Solids</i> , 2000, 61, 153-157.	1.9	5
121	Metal-insulator transition in disordered systems from the one-body density matrix. <i>Physical Review B</i> , 2017, 95, .	1.1	5
122	From the dipole of a crystallite to the polarization of a crystal. <i>Journal of Chemical Physics</i> , 2021, 154, 050901.	1.2	5
123	Faraday law, oxidation numbers, and ionic conductivity: The role of topology. <i>Journal of Chemical Physics</i> , 2021, 155, 244503.	1.2	5
124	Drude weight in systems with open boundary conditions. <i>Physical Review B</i> , 2020, 102, .	1.1	4
125	Chern number and orbital magnetization in ribbons, polymers, and single-layer materials. <i>Physical Review B</i> , 2020, 101, .	1.1	4
126	Microscopic electronic screening in semiconductors. , 1985, , 183-194.		3

#	ARTICLE	IF	CITATIONS
127	Neglecting local-field effects in the band-offset problem. Journal of Physics Condensed Matter, 1990, 2, 10217-10222.	0.7	3
128	N-representability and density-functional construction in curvilinear coordinates. Solid State Communications, 1998, 106, 763-768.	0.9	3
129	Why are insulators insulating and metals conducting?. Europhysics News, 2003, 34, 92-94.	0.1	3
130	Macroscopic polarization in crystalline dielectrics. Computational and Theoretical Chemistry, 2004, 709, 201-205.	1.5	3
131	Macroscopic Dielectric Polarization: Hartree-Fock Theory. Lecture Notes in Quantum Chemistry II, 1996, , 273-288.	0.3	3
132	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.	0.7	2
133	Bulk excitons in solid neon: Theory. Physical Review B, 1980, 21, 4889-4891.	1.1	2
134	Quantum mechanism of polarization in perovskites. Ferroelectrics, 1995, 164, 153-159.	0.3	2
135	Theory of longitudinal and transverse nonlinear dc conductivity. Physical Review Research, 2022, 4, .	1.3	2
136	Ionized impurity scattering in semimetals. Physical Review B, 1980, 22, 3935-3938.	1.1	1
137	Screening of a point charge in semiconductors and insulators. Physical Review B, 1988, 38, 818-818.	1.1	1
138	What makes an insulator different from a metal?. AIP Conference Proceedings, 2000, , .	0.3	0
139	Dielectric Polarization of Materials: A Modern View. Materials Research Society Symposia Proceedings, 2001, 677, 611.	0.1	0
140	Electrical Polarization and Orbital Magnetization: The Position Operator Tamed. , 2018, , 1-31.		0
141	Electrical Polarization and Orbital Magnetization: The Position Operator Tamed. , 2020, , 151-181.		0
142	Reply to "Comment on "Magnetic circular dichroism versus orbital magnetization" ". Physical Review Research, 2020, 2, .	1.3	0
143	Adiabatic electronic flux in molecules and in condensed matter. Journal of Chemical Physics, 2022, 156, .	1.2	0