

**RAFFAELE RESTA – LISTA DELLE PUBBLICAZIONI***(Gennaio 2012)***A – Lavori di rassegna, libri**

- A-1 A. Baldereschi e R. Resta,  
*Dielectric properties and lattice dynamics of semiconductors*,  
in: *Ab-Initio Calculation of Phonon Spectra*, a cura di J. T. Devreese et al.  
(Plenum Publishing, New York, 1983), pag. 1.
- A-2 R. Resta,  
*Dielectric properties of semiconductors*,  
in: *Proceedings of the 6th General Conference of the European Physical Society  
“Trends in Physics”*, a cura di J. Janta e J. Pantoflíček  
(Polygrafia, Praga, 1984), pag. 479.
- A-3 R. Resta,  
*Microscopic electronic screening in semiconductors*,  
in: *Festkörperprobleme*, vol. XXV, a cura di P. Grosse  
(Vieweg, Braunschweig, 1985). pag. 183.
- A-4 R. Resta,  
*Shallow impurity states in semiconductors: Theoretical aspects*,  
in: *Crystalline Semiconducting Materials and Devices*, a cura di P. N. Butcher, N.  
H. March e M. P. Tosi  
(Plenum Publishing, New York, 1986), pag. 217.
- A-5 A. Baldereschi e R. Resta (curatori),  
*Shallow Impurity Centers in Semiconductors*  
(North-Holland, Amsterdam, 1987).
- A-6 S. Baroni, R. Resta e A. Baldereschi,  
*Band offsets at semiconductor heterojunctions: bulk or interface properties?*,  
in: *Band Structure Engineering in Semiconductor Microstructures*, a cura di R.A.  
Abram e M. Jaros, NATO ASI Series B vol. 189  
(Plenum Publishing, New York, 1989), pag. 51.
- A-7 S. Baroni, R. Resta, A. Baldereschi e M. Peressi,  
*Can we tune the band offsets at semiconductor heterojunctions?*  
in: *Spectroscopy of Semiconductor Microstructures*, a cura di G. Fasol, A. Fasolino  
e P. Lugli, NATO ASI Series B, vol. 206  
(Plenum, New York, 1989), pag. 251.

- A-8 A. Baldereschi, M. Peressi, S. Baroni e R. Resta,  
*Semiconductor interfaces*,  
in: *Proceedings of the International School of Physics "Enrico Fermi", Course CXVII, Semiconductor Superlattices and Interfaces*, a cura di A. Stella e L. Miglio (North-Holland, Amsterdam, 1993), pag. 59.
- A-9 L. Colombo, R. Resta e S. Baroni,  
*Chemistry, interface features and strain: How do they affect the valence band offset at Si/Ge interfaces?*  
in *Proceedings of the 12<sup>th</sup> General Conference of the Condensed Matter Division of the European Physical Society*, a cura di B. Velický, V. Vorlíček, e K. Závěta, *Physica Scripta* **T45**, 181 (1992).
- A-10 S. Baroni, M. Peressi, R. Resta e A. Baldereschi,  
*Theory of band offsets at semiconductor heterojunctions*,  
in: *Proceedings of the 21th International Conference on the Physics of Semiconductors*, a cura di Ping Jiang e Hou-Zhi Zheng (World Scientific, Singapore, 1993), pag. 689.
- A-11 A. Baldereschi, R. Resta, M. Peressi, S. Baroni, e K. Mäder,  
*Engineering of semiconductor heterostructures by ultrathin control layers*,  
in: *Semiconductor Interfaces at the Sub-Nanometer Scale*, a cura di H.W. Salemink e M.D. Pashley, NATO ARW Series E, vol. 243 (Kluwer Academic, Dordrecht, 1993), pag. 89.
- A-12 R. Resta,  
*Macroscopic polarization in crystalline dielectrics: The geometric phase approach*,  
*Rev. Mod. Phys.* **66**, 899 (1994).
- A-13 R. Resta,  
*Che cos'è la polarizzazione dielettrica macroscopica?*  
*Il Nuovo Saggiatore* **9** (5/6), 79 (1993).
- A-14 R. Resta,  
*Computation in condensed matter physics*,  
*Memorie della Società Astronomica Italiana* **64**, 869 (1993).
- A-15 M. Peressi, L. Colombo, A. Baldereschi, R. Resta, e S. Baroni,  
*Band offset engineering at semiconductor heterojunctions*,  
*Society of Photo-Optical Instrumentation Engineering Proceedings Series* **1985**, 84 (1993).
- A-16 R. Resta,  
*Macroscopic dielectric polarization: Hartree-Fock theory*,  
in: *Quantum-Mechanical Ab-initio Calculation of the Properties of Crystalline Materials*, a cura di C. Pisani; *Lecture Notes in Chemistry*, Vol. **67** (Springer, Berlin, 1996), p. 273.

- A-17 R. Resta,  
*Berry Phase in Electronic Wavefunctions*,  
Lecture Notes for the “Troisième Cycle de la Physique en Suisse Romande” (Lausanne, 1996). Available online (194K) at the URL:  
[http://www-dft.ts.infn.it/~resta/publ/notes\\_trois.ps.gz](http://www-dft.ts.infn.it/~resta/publ/notes_trois.ps.gz).
- A-18 R. Resta,  
*Polarization as a Berry phase*,  
Europhys. News **28**, 18 (1997).
- A-19 R. Resta,  
*Topics in Polarization Theory*,  
in: *Advances in Computational Materials Science*, a cura di V. Fiorentini e F. Meloni (Società Italiana di Fisica, Bologna, 1998), pag.3.
- A-20 R. Resta,  
*Manifestations of Berry’s phase in molecules and in condensed matter*,  
J. Phys.: Condens. Matter **12**, R107 (2000).
- A-21 R. Resta,  
*Berry’s Phase and Geometric Quantum Distance: Macroscopic Polarization and Electron Localization*,  
Lecture Notes for the “Troisième Cycle de la Physique en Suisse Romande” (Lausanne, 2000). Available online (376K) at the URL:  
<http://www-dft.ts.infn.it/~resta/publ/notes2000.ps.gz>.
- A-22 R. Resta,  
*Insulators and metals*,  
in: *Electrons and Photons in Solids*, a cura di G. Grosso, G. La Rocca e M. P. Tosi (Quaderni della Scuola Normale Superiore, Pisa, 2001), pag. 357.
- A-23 R. Resta,  
*Why are insulators insulating and metals conducting?*,  
J. Phys.: Condens. Matter **14**, R625 (2002).
- A-24 R. Resta,  
*Ab-initio simulation of the properties of ferroelectric materials*,  
Modelling and Simulation in Materials Science and Engineering **11**, R69 (2003).
- A-25 R. Resta,  
*Why are insulators insulating and metals conducting?*,  
Europhys. News **34**, 92 (2003).
- A-26 R. Resta,  
*Geometrical phase and polarization in solids*,  
in: *Encyclopedia of Condensed Matter Physics*, G. F. Bassani, G. L. Liedl, and P. Wyder, editors (Elsevier, 2005), p. 267.

- A-27 D. Vanderbilt, R. Resta,  
*Quantum electrostatics of insulators – Polarization, Wannier functions, and electric fields*,  
in: *Conceptual foundations of materials: A standard model for ground- and excited-state properties*, S.G. Louie and M.L. Cohen, eds.  
(Elsevier, 2006), p. 139.
- A-28 R. Resta, D. Vanderbilt,  
*Theory of polarization: A modern approach*,  
in: *Physics of Ferroelectrics: a Modern Perspective*,  
Topics in Applied Physics v. **105**  
Ch. H. Ahn, K. M. Rabe, and J.-M. Triscone, eds.  
(Springer-Verlag, 2007), p. 31.
- A-29 R. Resta,  
*Charge states in transition*,  
Nature **453**, 735 (2008).
- A-30 R. Resta,  
*Electrical polarization and orbital magnetization: the modern theories*,  
J. Phys.: Condens. Matter **22** 123201 (2010).
- A-31 R. Resta,  
*The insulating state of matter: a geometrical theory*,  
Eur. Phys. J. B **79**, 121 (2011).

**B – Lavori originali**

- B-1 L. Piela, L. Pietronero e R. Resta,  
*Electron band structure of solid methane: Ab initio calculation*,  
Phys. Rev. B **7**, 5321 (1973).
- B-2 L. A. Gomez, G. Pastori-Parravicini e R. Resta,  
*Valence band structure and Davydov splittings in solid ortho-hydrogen*,  
J. Phys. C **6**, 1926 (1973).
- B-3 F. Bassani, L. Pietronero e R. Resta,  
*Band structure of solid HF*,  
J. Phys. C **6**, 2133 (1973).
- B-4 L. Piela, L. Pietronero e R. Resta,  
*Electron band structure of solid methane: Inclusion of intermolecular selfconsistency in calculations*,  
Phys. Rev. B **9**, 5332 (1974).
- B-5 V. dello Iacovo, L. Resca e R. Resta,  
*Valence energy bands of solid hydrogen in h.c.p. structure: Ab-initio LCMO calculation*,  
Phys. Status Solidi B **69**, 127 (1975).
- B-6 G. Grosso, G. Pastori-Parravicini e R. Resta,  
*Isotropic Compton profile of LiH in the tight-binding approximation*,  
Phys. Status Solidi B **73**, 371 (1976).
- B-7 R. Moccia, R. Resta e M. Zandomeneghi,  
*Bound state properties of  $H_2$  by the many-body Green's function method*,  
Chem. Phys. Lett. **37**, 556 (1976).
- B-8 N. Erre e R. Resta,  
*The use of electron-atom scattering phase shifts in conduction band calculations: Application to solid argon*  
J. Phys. C **9**, 2331 (1976).
- B-9 L. Resca e R. Resta,  
*Energy bands in cubic ice: Ab-initio calculation using the method of linear combination of molecular orbitals*,  
Phys. Status Solidi B **81**, 129 (1977).
- B-10 R. Resta,  
*A note on the many-valley effective mass theory*,  
J. Phys. C **10**, L179 (1977).
- B-11 R. Resta,  
*Thomas-Fermi dielectric screening in semiconductors*,  
Phys. Rev. B **16**, 2717 (1977).

- B-12 S. Natalizi e R. Resta,  
*The use of electron-atom scattering phase shifts in conduction band calculations: Solid neon*,  
J. Phys. C **10**, L477 (1977).
- B-13 R. Resta,  
*Quantum defect theory of excitons: Solid neon*,  
Phys. Status Solidi B **86**, 627 (1978).
- B-14 F. Cornolti e R. Resta,  
*Nonlinear impurity screening in semiconductors*,  
Phys. Rev. B **17**, 3239 (1978).
- B-15 L. Resca, R. Resta e S. Rodriguez,  
*Electronic excitations of the rare gases in the solid phase*,  
Solid State Commun. **26**, 849 (1978).
- B-16 R. Resta,  
*Study of the correlation holes: I. Number-sum rules and the infinite system*,  
Int. J. Quantum Chem. **14**, 171 (1978).
- B-17 L. Resca, R. Resta e S. Rodriguez,  
*Nonstructural theory of the exciton states in solid rare gases*,  
Phys. Rev. B **18**, 696 (1978).
- B-18 L. Resca, R. Resta e S. Rodriguez,  
*Core excitons in solid rare gases: Nonstructural theory*,  
Phys. Rev. B **18**, 702 (1978).
- B-19 L. Resca e R. Resta,  
*Large binding due to dispersive screening and Bloch function interference in many-valley semiconductors*,  
Solid State Commun. **29**, 275 (1979).
- B-20 L. Resca e R. Resta,  
*Rydberg states in condensed matter*,  
Phys. Rev. B **19**, 1683 (1979).
- B-21 R. Resta,  
*Dielectric behavior of a doped semiconductor*,  
Phys. Rev. B **19**, 3022 (1979).
- B-22 L. Resca e R. Resta,  
*Ionized impurity scattering in semiconductors*,  
Phys. Rev. B **20**, 3254 (1979).
- B-23 L. Resca e R. Resta,  
*Shallow-deep instabilities of donor impurity levels and excitons in many-valley semiconductors*,  
Phys. Rev. Lett. **44**, 1340 (1980).

- B-24 E. Doni, L. Resca, R. Resta e R. Girlanda,  
*Relationships between the semiempirical and the Hartree-Fock methods in band structure calculations*,  
Solid State Commun. **34**, 461 (1980).
- B-25 L. Resca e R. Resta,  
*Bulk excitons in solid neon: Theory*,  
Phys. Rev. B **21**, 4889 (1980).
- B-26 L. Resca e R. Resta,  
*Ionized impurity scattering in semimetals*,  
Phys. Rev. B **22**, 3935 (1980).
- B-27 R. Cimiraglia e R. Resta,  
*Study of correlation holes: II. CI calculations on model polyatomic systems*,  
Int. J. Quantum Chem. **19**, 301 (1981).
- B-28 R. Resta e A. Baldereschi,  
*Dielectric matrices and local fields in polar semiconductors*,  
Phys. Rev. B **23**, 6615 (1981).
- B-29 R. Resta e A. Baldereschi,  
*Local-field effects and zone-center phonons in Si, Ge, GaAs and ZnSe*,  
Phys. Rev. B **24**, 4839 (1981).
- B-30 L. Resca, R. Resta e S. Rodriguez,  
*Ionized impurity scattering and dielectric enhancement of mobility in semiconductors and semimetals*,  
in: *Recent Developments in Condensed Matter Physics*, a cura di J. T. Devreese et al.  
(Plenum Publishing, New York, 1981), vol. **3**, pag. 21.
- B-31 R. Resta e A. Baldereschi,  
*Local-field effects and zone-center phonons in polar and covalent cubic semiconductors*,  
Journal de Physique **42**, C6-661 (1981).
- B-32 L. Resca, R. Resta e H. B. Shore,  
*Real-space equation for single-donor impurities and core excitons in many-valley semiconductors*,  
Phys. Rev. B **25**, 4031 (1982).
- B-33 L. Resca e R. Resta,  
*Single-donor impurities and core excitons in many-valley semiconductors*,  
Phys. Rev. B **25**, 4038 (1982).
- B-34 R. Resta,  
*Local-field effects and phonon screening in polar semiconductors*,  
Phys. Rev. B **27**, 3620 (1983).

- B-35 K. Kunc e R. Resta,  
*External fields in the selfconsistent theory of electronic states: A new method for direct evaluation of macroscopic and microscopic dielectric response*,  
Phys. Rev. Lett. **51**, 686 (1983).
- B-36 A. Fleszar e R. Resta,  
*Dielectric matrices in semiconductors: A direct approach*,  
Phys. Rev. B **31**, 5305 (1985).
- B-37 S. Baroni e R. Resta,  
*Ab-initio calculation of the Raman tensor in silicon*,  
in: *Proceedings of the 2nd International Conference on Phonon Physics*,  
a cura di J. Kollàr et al. (World Scientific, Singapore, 1985), pag. 946.
- B-38 A. Fleszar e R. Resta,  
*Interplanar and interatomic force constants in silicon and germanium in the adiabatic bond-charge model*,  
in: *Proceedings of the 2nd International Conference on Phonon Physics*,  
a cura di J. Kollàr et al. (World Scientific, Singapore, 1985), pag. 583.
- B-39 A. Fleszar, K. Kunc, R. Resta e E. Tosatti,  
*Crucial role of exchange and correlation in lattice dynamics of germanium*,  
in: *Proceedings of the 2nd International Conference on Phonon Physics*,  
a cura di J. Kollàr et al. (World Scientific, Singapore, 1985), pag. 930.
- B-40 S. Baroni e R. Resta,  
*Ab-initio calculation of the low-frequency Raman cross-section in silicon*,  
Phys. Rev. B **33**, 5969 (1986).
- B-41 S. Baroni e R. Resta,  
*Ab-initio calculation of the macroscopic dielectric constant of silicon*,  
Phys. Rev. B **33**, 7017 (1986).
- B-42 A. Fleszar e R. Resta,  
*Real-space force constants for lattice dynamics in silicon and germanium*,  
Phys. Rev. B **34**, 7140 (1986).
- B-43 R. Resta e K. Kunc,  
*Self-consistent theory of electronic states and dielectric response in semiconductors*,  
Phys. Rev. B **34**, 7146 (1986).
- B-44 A. Qteish e R. Resta,  
*Microscopic atomic structure and stability of Si-Ge solid solutions*,  
Phys. Rev. B **37**, 1308 (1988).
- B-45 A. Baldereschi, S. Baroni e R. Resta,  
*Band offsets at GaAs/AlAs interfaces: A model and first-principles calculations*,  
Vuoto **17**, 10 (1988).

- B-46 A. Qteish e R. Resta,  
*Thermodynamic properties of Si-Ge alloys*,  
Phys. Rev. B **37**, 6983 (1988).
- B-47 R. Resta,  
*Screening of a point charge in semiconductors and insulators*,  
Phys. Rev. B **38**, 818 (1988).
- B-48 A. Baldereschi, S. Baroni e R. Resta,  
*Band offsets in lattice matched heterojunctions: A model and first-principles calculations for GaAs/AlAs*,  
Phys. Rev. Lett. **61**, 734 (1988).
- B-49 R. Resta, S. Baroni e A. Baldereschi,  
*Theory of band offsets at semiconductor heterojunctions: An ab-initio linear response approach*,  
Superlattices and Microstructures **6**, 31 (1989).
- B-50 S. Baroni, R. Resta e A. Baldereschi,  
*Electronic structure of polar interfaces from linear-response theory*,  
in: *Proceedings of the 19th International Conference on the Physics of Semiconductors*, a cura di W. Zawadzky  
(Institute of Physics, Polish Academy of Sciences, Varsavia, 1988), pag. 525.
- B-51 R. Resta, A. Baldereschi e S. Baroni,  
*Electronic properties of isovalent and heterovalent semiconductor interfaces*,  
Journal de Chimie Physique **86**, 789 (1989).
- B-52 A. Qteish e R. Resta,  
*Ab-initio calculation of the phase diagram and microscopic structure of semiconductor binary alloys*,  
Journal de Chimie Physique **86**, 889 (1989).
- B-53 A. Qteish e R. Resta,  
*The electronic structure properties of Si-Ge alloys*,  
Preprint SISSA (1989).
- B-54 S. de Gironcoli, S. Baroni e R. Resta,  
*Piezoelectric properties of III-V semiconductors from first-principle linear-response theory*,  
Phys. Rev. Lett. **62**, 2853 (1989).
- B-55 A. Baldereschi, G. Ortíz e R. Resta,  
*Charge transfer vs. energy pinning at semiconductor interfaces*,  
Helv. Phys. Acta **62**, 838 (1989).
- B-56 M. Peressi, S. Baroni, A. Baldereschi e R. Resta,  
*Valence-band offset at InP/Ga<sub>0.47</sub>In<sub>0.53</sub>As lattice-matched heterojunctions*,  
Helv. Phys. Acta **62**, 862 (1989).

- B-57 P. Giannozzi, S. de Gironcoli e R. Resta,  
*The macroscopic polarization of a zone-center transverse mode*,  
in: *Phonons 89*, a cura di S. Hunkliger, W. Ludwig e G. Weiss (World Scientific,  
Singapore, 1990), pag. 205.
- B-58 R. Resta, L. Colombo e S. Baroni,  
*Absolute deformation potentials in semiconductors*,  
in: *Phonons 89*, a cura di S. Hunkliger, W. Ludwig e G. Weiss (World Scientific,  
Singapore, 1990), pag. 208.
- B-59 M. Posternak, A. Baldereschi, A. Catellani e R. Resta,  
*Ab-initio study of the spontaneous polarization of pyroelectric BeO*,  
Phys. Rev. Lett. **64**, 1777 (1990).
- B-60 G. Ortíz, R. Resta e A. Baldereschi,  
*Neglecting local-field effects in the band-offset problem*,  
J. Phys.: Condens. Matter **2**, 10217 (1990).
- B-61 R. Resta, L. Colombo e S. Baroni,  
*Absolute deformation potentials in semiconductors*,  
Phys. Rev. B **41**, 12358 (1990).; **43**, 14273(Erratum) (1991).
- B-62 S. de Gironcoli, S. Baroni e R. Resta,  
*Piezoelectricity in III-V and II-VI semiconductors: a systematic ab-initio calculation*,  
Ferroelectrics **111**, 19 (1990).
- B-63 R. Resta, M. Posternak, A. Baldereschi e A. Catellani,  
*Spontaneous polarization from first principles: pyroelectric BeO*,  
Ferroelectrics **111**, 15 (1990).
- B-64 M. Peressi, S. Baroni, A. Baldereschi e R. Resta,  
*Electronic structure of InP/Ga<sub>0.47</sub>In<sub>0.53</sub>As interfaces*,  
Phys. Rev. B **41**, 12106 (1990).
- B-65 J.T. McKinley, Y. Hwu, B.E.C. Koltenbah, G. Margaritondo, S. Baroni e R. Resta,  
*Control of Ge homojunction band offsets via ultrathin Ga-As dipole layers*,  
J. Vac. Sci. Techn. A **9**, 917 (1991).
- B-66 M. Peressi, S. Baroni, R. Resta e A. Baldereschi,  
*Tuning band offsets at semiconductor interfaces by intralayer deposition*,  
Phys. Rev. B **43**, 7347 (1991).
- B-67 L. Colombo, R. Resta e S. Baroni,  
*Valence band offsets at strained Si/Ge interfaces*,  
Phys. Rev. B **44**, 5572 (1991).

- B-68 R. Resta  
*Deformation-potential theorem in metals and in dielectrics*,  
Phys. Rev. B **44**, 11035 (1991).
- B-69 M. Marsi, S. La Rosa, Y. Hwu, F. Gozzo, C. Coluzza, A. Baldereschi, G. Margaritondo, J.T. McKinley, S. Baroni, e R. Resta,  
*Microscopic manipulation of homojunction band lineups*,  
J. Appl. Phys. **71**, 2048 (1992).
- B-70 J.T. McKinley, Y. Hwu, B.E.C. Koltenbah, G. Margaritondo, S. Baroni e R. Resta,  
*Control of Ge homojunction band offsets via ultrathin Ga-As dipole layers*,  
Appl. Surf. Sci. **56-58**, 762 (1992).
- B-71 A. Baldereschi, M. Posternak, e R. Resta,  
*Ab-initio study of the spontaneous polarization of pyroelectric BeO: Reply to a Comment*,  
Phys. Rev. Lett. **69**, 390 (1992).
- B-72 G. Biasiol, L. Sorba, G. Bratina, R. Nicolini, A. Franciosi, M. Peressi, S. Baroni, R. Resta, e A. Baldereschi,  
*Microscopic capacitor and neutral interfaces in III-V/IV/III-V semiconductor heterostructures*,  
Phys. Rev. Lett. **69**, 1283 (1992).
- B-73 R. Resta,  
*Theory of the electric polarization in crystals*,  
Ferroelectrics **136**, 51 (1992).
- B-74 A. Dal Corso, S. Baroni, R. Resta, e S. de Gironcoli,  
*Ab-initio calculation of phonon dispersions in II-VI semiconductors*,  
Phys. Rev. B **47**, 3588 (1993).
- B-75 R. Resta, M. Posternak, e A. Baldereschi,  
*Towards a quantum theory of polarization in ferroelectrics: The case of KNbO<sub>3</sub>*,  
Phys. Rev. Lett. **70**, 1010 (1993).
- B-76 A. Dal Corso, R. Resta, e S. Baroni,  
*Nonlinear piezoelectricity in CdTe*,  
Phys. Rev. B **47**, 16252 (1993).
- B-77 R. Resta, M. Posternak, e A. Baldereschi,  
*First-principles theory of polarization in ferroelectrics*,  
Mater. Res. Soc. Symp. Proc. **291**, 647 (1993).
- B-78 R. Resta,  
*Macroscopic polarization as a geometric quantum phase*  
Europhys. Lett. **22**, 133 (1993).

- B-79 M. Peressi, L. Colombo, R. Resta, S. Baroni, e A. Baldereschi,  
*Structural and electronic properties of strained Si/GaAs heterostructures*,  
Phys. Rev. B **48**, 12047 (1993).
- B-80 A. Dal Corso, S. Baroni, e R. Resta,  
*Density-functional theory of the dielectric constant: Gradient-corrected calculation for silicon*,  
Phys. Rev. B **49**, 5323 (1994).
- B-81 R. Nicolini, L. Vanzetti, G. Mula, G. Bratina, L. Sorba, A. Franciosi, M. Peressi, S. Baroni, R. Resta, A. Baldereschi, J.E. Angelo e W.W. Gerberich,  
*Local interface composition and band discontinuities in heterovalent heterostructures*,  
Phys. Rev. Lett. **72**, 294 (1994).
- B-82 R. Resta,  
*Modern theory of polarization in ferroelectrics*,  
Ferroelectrics, **151**, 49 (1994).
- B-83 A. Dal Corso e R. Resta,  
*Density-functional theory of macroscopic stress: Gradient-corrected calculations for crystalline Se*,  
Phys. Rev. B **50**, 4327 (1994).
- B-84 M. Posternak, R. Resta, e A. Baldereschi,  
*Role of covalent bonding in the polarization of perovskite oxides: The case of  $\text{KNbO}_3$* ,  
Phys. Rev. B **50**, 8911 (1994).
- B-85 A. Dal Corso, M. Posternak, R. Resta, e A. Baldereschi,  
*Ab-initio study of piezoelectricity and spontaneous polarization in ZnO*,  
Phys. Rev. B **50**, 10715 (1994).
- B-86 R. Resta, M. Posternak, e A. Baldereschi,  
*Quantum mechanism of polarization in perovskites*,  
Ferroelectrics **164**, 153 (1995).
- B-87 R. Resta e S. Sorella,  
*Many-body effects on polarization and dynamical charges in a partly covalent polar insulator*,  
Phys. Rev. Lett. **74**, 4738 (1995).
- B-88 S. Massidda, R. Resta, M. Posternak, e A. Baldereschi,  
*Polarization and dynamical charge of ZnO within different one-particle schemes*,  
Phys. Rev. B **52**, 16977 (1995).

- B-89 R. Resta, S. Massidda, M. Posternak, e A. Baldereschi,  
*Polarization, dynamical charge, and bonding in partly covalent polar insulators*,  
Mater. Res. Soc. Symp. Proc., **408**, 9 (1996).
- B-90 R. Resta,  
*Role of covalence and of correlation in the dielectric polarization of oxides*,  
Ferroelectrics **194**, 1 (1997).
- B-91 R. Resta,  
*Density-polarization-functional theory and long-range correlation in dielectrics*,  
Phys. Rev. Lett. **77**, 2265 (1996).
- B-92 S. Picozzi, S. Massidda, A. Continenza, and R. Resta,  
*Highly tunable valence-band offset at the (111) Si/Si homojunction via a CaF monolayer saturated with H*,  
Phys. Rev. B **55**, 16318 (1997).
- B-93 R. Resta,  
*Density-polarization-functional theory and long-range correlation in dielectrics: Reply to Comments*,  
Phys. Rev. Lett. **78**, 2030 (1997).
- B-94 A. Ruini, R. Resta, and S. Baroni,  
*Dynamical-charge neutrality at a crystal surface*,  
Phys. Rev. B **57**, 5742 (1998).
- B-95 M Posternak, A. Baldereschi, H. Krakauer, and R. Resta,  
*Non-nominal value of the dynamical effective charge in alkaline-earth oxides*,  
Phys. Rev. B **55**, R15983 (1997).
- B-96 A. Ruini, R. Resta, and S. Baroni,  
*The effect of interface morphology on Schottky barrier heights: A case study on Al/GaAs(001)*,  
Phys. Rev. B **56**, 14921 (1997).
- B-97 S. Dall'Olio, R. Dovesi, and R. Resta,  
*Spontaneous polarization as a Berry phase of the Hartree-Fock wavefunction: The case of KNbO<sub>3</sub>*,  
Phys. Rev. B **56**, 10105 (1997).
- B-98 A.I. Al-Sharif, R. Resta, and C.J. Umrigar,  
*Evidence of physical reality in the Kohn-Sham potential: The case of atomic Ne*,  
Phys. Rev. A **57**, 2466 (1998).
- B-99 L. Fu, E. Yaschenko, L. Resca, and R. Resta  
*Hartree-Fock approach to macroscopic polarization: Dielectric constant and dynamical charges of KNbO<sub>3</sub>*,  
Phys. Rev. B **57**, 6967 (1998).

- B-100 R. Resta,  
*Quantum mechanical position operator in extended systems*,  
Phys. Rev. Lett. **80**, 1800 (1998).
- B-101 E. Yaschenko, L. Fu, L. Resca, and R. Resta,  
*Macroscopic polarization as a discrete Berry phase of the Hartree-Fock wavefunction: The single-point limit*,  
Phys. Rev. B **58**, 1222 (1998).
- B-102 L. De Santis and R. Resta,  
*N-representability and density-functional construction in curvilinear coordinates*,  
Solid State Commun. **106**, 763 (1998).
- B-103 R. Resta,  
*The quantum mechanical position operator and the polarization problem*,  
in: *First-Principles Calculations for Ferroelectrics: Fifth Williamsburg Workshop*,  
R.E. Cohen, ed. (AIP, Woodbury, New York, 1998), p. 174;  
also available as preprint cond-mat/9802004.
- B-104 L. Fu, E. Yaschenko, L. Resca, and R. Resta,  
*Hartree-Fock studies of the ferroelectric perovskites*,  
in: *First-Principles Calculations for Ferroelectrics: Fifth Williamsburg Workshop*,  
R.E. Cohen, ed. (AIP, Woodbury, New York, 1998), p. 107;  
also available as preprint cond-mat/9803002.
- B-105 S. Massidda, M Posternak, A. Baldereschi, and R. Resta,  
*Non-cubic behavior of antiferromagnetic transition-metal monoxides with the rock-salt structure*,  
Phys. Rev. Lett. **82**, 430 (1999).
- B-106 L. De Santis and R. Resta,  
*Surface reconstructions and bonding via the electron localization function: The case of Si(001)*,  
Solid State Commun. **111**, 583 (1999).
- B-107 R. Resta and S. Sorella,  
*Electron localization in the insulating state*,  
Phys. Rev. Lett. **82**, 370 (1999).
- B-108 L. Fu, E. Yaschenko, L. Resca, and R. Resta,  
*Hartree-Fock studies of the surface properties of BaTiO<sub>3</sub>*,  
Phys. Rev. B **60**, 2697 (1999).
- B-109 L. Fu, E. Yaschenko, L. Resca, and R. Resta,  
*Polarization properties of KNbO<sub>3</sub>: Comparison between Hartree-Fock and density-functional calculations*,  
Solid State Commun. **112**, 465 (1999).

- B-110 R. Resta,  
*Dynamical charges in oxides: Recent advances*,  
J. Phys. Chem. Solids **61**, 153 (2000).
- B-111 L. De Santis and R. Resta,  
*Electron localization at metal surfaces*,  
Surf. Sci. **450**, 126 (2000).
- B-112 R. Resta,  
*Macroscopic polarization from electronic wavefunctions*,  
Int. J. Quantum. Chem. **75**, 599 (1999).
- B-113 A. I. Alsharif, A. Qteish, and R. Resta,  
*A simple method for constructing highly accurate atomic Kohn–Sham potentials*,  
Phys. Rev. A **60**, 3541 (1999).
- B-114 R. Resta,  
*What makes an insulator different from a metal?*  
in: *Fundamental Physics of Ferroelectrics*, R.E. Cohen and K. Rabe, editors (AIP,  
Woodbury, New York, 2000), p. 67;  
also available as preprint cond-mat/0003014.
- B-115 P. Umari, A. Dal Corso, and R. Resta,  
*What happens inside a polarized dielectric?*,  
(inviato per la pubblicazione).
- B-116 A. Pasquarello and R. Resta,  
*Dynamical monopoles and dipoles in a condensed molecular system: The case of  
liquid water*,  
Phys. Rev. B **68**, 174302 (2003).
- B-117 P. Umari, A. Dal Corso, and R. Resta,  
*Inside dielectrics: Microscopic and macroscopic polarization*,  
in: *Fundamental Physics of Ferroelectrics: 2001 Williamsburg Workshop*, H. Krakauer,  
ed. (AIP, Woodbury, New York, 2001), p. 107.
- B-118 C. Sgiarovello, M. Peressi, and R. Resta,  
*Electron localization in the insulating state: Application to crystalline semiconduc-  
tors*,  
Phys. Rev. B **64**, 115202 (2001).
- B-119 R. Resta,  
*Dielectric polarization of materials: A modern view*,  
Mater. Res. Soc. Symp. Proc. **677** p. AA6.1.1 (2001).
- B-120 R. Resta and L. Resca,  
*Comment on “Electrostatic screening near semiconductor surfaces”*,  
Phys. Rev. B **65**, 047301 (2002).

- B-121 A. Pasquarello and R. Resta,  
*A generalization of the effective-charge concept: Dynamical multipoles in molecular solids and liquids*,  
in: *Fundamental Physics of Ferroelectrics 2002*, R. E. Cohen and T. Egami eds.  
(AIP, Woodbury, 2002), p. 198.
- B-122 R. Resta,  
*Comment on "Locality and topology in the molecular Aharonov-Bohm effect"*,  
Phys. Rev. Lett. **91**, 048901 (2003).
- B-123 V. Srinivasan, R. Gebauer, R. Resta, and R. Car,  
*PbTiO<sub>3</sub> at finite temperature: An ab-initio molecular dynamics study*,  
in: *Fundamental Physics of Ferroelectrics 2003*, P. K. Davies and D. J. Singh eds.  
(AIP, Woodbury, 2003), p. 168.
- B-124 R. Resta,  
*Macroscopic polarization in crystalline dielectrics*,  
J. Molecular Structure (Theochem) **709**, 201 (2004).
- B-125 K. N. Kudin, R. Car, and R. Resta,  
*Longitudinal polarizability of long polymeric chains: Quasi-one-dimensional electrostatics as the origin of slow convergence*,  
J. Chem. Phys. **122**, 134907 (2005).
- B-126 R. Resta, D. Ceresoli, T. Thonhauser, and D. Vanderbilt,  
*Orbital magnetization in extended systems*,  
ChemPhysChem **6**, 1815 (2005).
- B-127 R. Resta,  
*Electron Localization in the Quantum-Hall Regime*,  
Phys. Rev. Lett. **95**, 196805 (2005).
- B-128 T. Thonhauser, D. Ceresoli, D. Vanderbilt, R. Resta,  
*Orbital magnetization in periodic insulators*,  
Phys. Rev. Lett. **95**, 137205 (2005).
- B-129 M. Sharma, R. Resta, R. Car,  
*Intermolecular dynamical charge fluctuations in water: a signature of the H-bond network*,  
Phys. Rev. Lett. **95**, 187401 (2005).
- B-130 D. Ceresoli, T. Thonhauser, D. Vanderbilt, R. Resta,  
*Orbital magnetization in crystalline solids: Multi-band insulators, Chern insulators, and metals*,  
Phys. Rev. B, **74**, 024408 (2006).
- B-131 R. Resta,  
*Polarization fluctuations in insulators and metals: New and old theories merge*,  
Phys. Rev. Lett. **96**, 137601 (2006).

- B-132 R. Resta,  
*Kohn's theory of the insulating state: A quantum-chemistry viewpoint*,  
J. Chem. Phys. **124**, 104104 (2006).
- B-133 K. N. Kudin, R. Car, and R. Resta,  
*Berry phase approach to longitudinal dipole moments of infinite chains in electronic-structure methods with local basis sets*,  
J. Chem. Phys. **126**, 234101 (2007).
- B-134 M. Sharma, R. Resta, R. Car,  
*Dipolar correlations and the dielectric permittivity of water*,  
Phys. Rev. Lett. **98**, 247401 (2007).
- B-135 D. Ceresoli, R. Resta,  
*Orbital magnetization and Chern number in a supercell framework: Single  $\mathbf{k}$ -point formula*,  
Phys. Rev. B **76**, 012405 (2007).
- B-136 K. N. Kudin, R. Car, and R. Resta,  
*Quantization of the dipole moment and of the end charges in push-pull polymers*,  
J. Chem. Phys. **127**, 194902 (2007).
- B-137 I. Ponomareva, L. Bellaiche, R. Resta,  
*Relation between dielectric responses and polarization's fluctuations in ferroelectric nanostructures*,  
Phys. Rev. B **76**, 235403 (2007).
- B-138 I. Ponomareva, L. Bellaiche, R. Resta,  
*Dielectric anomalies in ferroelectric nanostructures*,  
Phys. Rev. Lett. **99**, 227601 (2007).
- B-139 T. Thonhauser, A.A. Mostofi, N. Marzari, R. Resta, D. Vanderbilt,  
*A converse approach to the calculation of NMR shielding tensors*,  
J. Chem. Phys. **131**, 101101 (2009).
- B-140 W. Chen, M. Sharma, R. Resta, G. Galli, R. Car,  
*Role of dipolar correlations in the infrared spectra of water and ice*,  
Phys. Rev. B **77**, 245114 (2008).
- B-141 R. Resta,  
*Macroscopic electrical polarization of materials (disordered and crystalline)*,  
J Phys.: Conference Series **117**, 012024 (2008).
- B-142 H. Raebiger, S. Lany, R. Resta, A. Zunger,  
*Oxidation numbers as social security numbers: Are they predictive or postdictive?*,  
<http://hdl.handle.net/10101/npre.2009.4012.1> (2009).

- B-143 G. L. Bendazzoli, S. Evangelisti, A. Monari, and R. Resta,  
*Kohn's localization in the insulating state: one-dimensional lattices,  
crystalline vs. disordered,*  
J. Chem. Phys. **133**, 064703 (2010).
- B-144 R. Resta,  
*Towards a bulk theory of flexoelectricity,*  
Phys. Rev. Lett. **105**, 127601 (2010).
- B-145 R. Resta,  
*Lyddane-Sachs-Teller relationship in linear magnetoelectrics,*  
Phys. Rev. Lett. **106**, 047202 (2011).
- B-146 R. Bianco and R. Resta,  
*Mapping topological order in coordinate space,*  
Phys. Rev. B **84**, 241106(R)(2011).
- B-147 R. Resta,  
*Zone-center dynamical matrix in magnetoelectrics,*  
Phys. Rev. B **84**, 214428 (2011).