CURRICULUM VITAE

Andrea Dal Corso

PRESENT ADDRESS

International School for Advanced Studies (SISSA-ISAS),
Via Bonomea 265,
I-34136, Trieste (Italy).
Tel.: +39 040 3787 428.
Fax.: +39 040 3787 249.
E-mail: dalcorso@sissa.it.

EDUCATION

- Born: 1965, Adria (Rovigo).
- High school: Liceo Scientifico "E. Majorana", Mirano (Venezia, Italy) 1979 – 84.
  "Maturità" degree: June 1984. Final vote: 60/60.
- University: Department of Physics, University of Padova, Padova (Italy) 1984 – 89.
  "Laurea" degree: March 1989. Final vote: 110/110 cum laude.
- Graduate studies: International School for Advanced Studies, Trieste (Italy) 1990 – 93.
  Master degree: April 1992. Final vote: 30/30 cum laude.
  PhD : October 1993. Final vote: approved cum laude.

PREVIOUS POSITIONS

- Postdoctoral Positions: IRRMA (Institut Romand de Recherche Numérique en Physique des Matériaux) and Institut de Physique Appliquée (EPFL). Lausanne 1993 – 1997.
- Senior Researcher: IRRMA (Institut Romand de Recherche Numérique en Physique des Matériaux) and Institut de Physique Appliquée (EPFL). Lausanne 1998.
- Temporary Researcher (3+3): SISSA – ISAS, International School for Advanced Studies. Trieste 1999 – 2002.
- Associate Professor: SISSA – ISAS, International School for Advanced Studies. Trieste 2002 –.
- National Scientific Habilitation to the role of Full Professor. Valid until 11/12/2019.

RESEARCH ACTIVITY AND PUBLICATIONS

My research activity is in the field of computational condensed matter, with the goal of extending the methods of electronic structure (based mainly on density functional theory) to deal with complex systems and novel properties. The `Quantum ESPRESSO` package [55,73] (see `http://www.quantum-espresso.org`) is a computer package for the investigation of the electronic structure of atoms, molecules, solids, and nanostructures, the optimization of the nuclear geometry and the calculation of the response to several perturbations [22]. Part of my activity aimed to improve this package [1,4,6,10,17,20,29,39,40,41,45,47,56,58,73]. I have generalized density functional perturbation theory to the ultrasoft pseudopotentials [10,29,47] and PAW [56]. In recent years, I have devoted a particular effort to the development of numerical methods for the study of relativistic effects such as spin-orbit coupling with plane waves and pseudopotentials [41,45,47,58,63,67,77]. I have developed and mantain a library of scalar and fully relativistic PAW and ultrasoft pseudopotentials (see `https://dalcorso.github.io/pslibrary`) [67] and I am investigating methods to parallelize and simplify the calculation of material properties (see `https://dalcorso.github.io/thermo_pw`) [68,70,71,72,76,77,78,80].

I have made or contributed to several applications to bulk materials [1,3,4,5,8,9,10,17,20,41, 47,53,63,65,66,70,71,72,76,77,78,79,80,81], molecules [60], transition and noble metal surfaces, clean and with adsorbates [21,23,24,27,30,32,37,38,43,46,49,68,74,75], and nanostructures such as metallic nanowires and nanocontacts [14,25,36,40,44,45,48,51,52,54,57,61,62,64,77].

These papers have been cited more than 23,000 times in the international literature (H index 36), Refs. [22,55,73] have more than 1000 quotes, Ref. [1,7,8,14,16,25,26,35,40,41,67,69] have 100 or more quotes, and other 13 papers have 50 or more quotes (source: ISI, Sep. 2020).
Selected publications: [1,20,29,39,41,47,49,56,58,67,70].

Papers

1. A. Dal Corso, S. Baroni, R. Resta, and S. de Gironcoli, "*Ab-initio* calculation of phonon dispersions in II-VI semiconductors", Phys. Rev. B **47**, 3588 (1993).

2. A. Dal Corso and E. Tosatti, "Face-dependent Hamaker constants and surface melting or non-melting of non-cubic crystals", Phys. Rev. B **47**, 9742 (1993).

3. A. Dal Corso, R. Resta, and S. Baroni, "Non linear piezoelectricity in CdTe", Phys. Rev. B **47**, 16252 (1993).

4. A. Dal Corso, S. Baroni and R. Resta, "Density-functional theory of the dielectric constant: gradient corrected calculation for silicon", Phys. Rev. B **49**, 5323 (1994).

5. A. Dal Corso and R. Resta, "Density-functional theory of macroscopic stress: Gradient-corrected calculations for crystalline Se", Phys. Rev. B **50**, 4327 (1994).

6. A. Dal Corso and F. Mauri, "Wannier and Bloch orbital computation of nonlinear susceptibility", Phys. Rev. B (Rapid Communication) **50**, 5756 (1994).

7. A. Dal Corso, M. Posternak, R. Resta and A. Baldereschi, "*Ab-initio* study of piezoelectricity and spontaneous polarization in ZnO", Phys. Rev. B **50**, 10715 (1994).

8. A. Dal Corso, A. Pasquarello, A. Baldereschi, and R. Car, "Generalized Gradient approximations to density functional theory: a comparative study for atoms and solids", Phys. Rev. B **53**, 1180 (1996).

9. A. Dal Corso, F. Mauri, and A. Rubio, "Density-functional theory of nonlinear optical susceptibility: Application to cubic semiconductors", Phys. Rev. B **53**, 15638 (1996).

10. A. Dal Corso, A. Pasquarello, and A. Baldereschi, "Density-functional perturbation theory for lattice dynamics with ultrasoft pseudopotentials", Phys. Rev. B (Rapid Communication) **56**, R11369 (1997).

11. P. Fernández, A. Dal Corso, F. Mauri, and A. Baldereschi, "First-Principle Wannier functions of silicon and gallium arsenide", Phys. Rev. B (Rapid Communication) **55**, R1909 (1997).

12. P. Fernández, A. Dal Corso, and A. Baldereschi, " Ab initio study of the dielectric properties of silicon and gallium arsenide using polarized Wannier functions", Phys. Rev. B (Rapid Communication) **58**, R7480 (1998).

13. C. Massobrio, A. Pasquarello, and A. Dal Corso, "Structural and electronic properties of small Cu_n clusters using generalized-gradient approximations within density functional theory", Jour. of Chem. Phys. **109**, 6626 (1998).

14. J.A. Torres, E. Tosatti, A. Dal Corso, F. Ercolessi, J.J. Kohanoff, F. Di Tolla, and J.M. Soler, "The puzzling stability of monatomic gold wires", Surface Science Letters **426**, L441 (1999).

15. F. Mauri and A. Dal Corso, "Vibrational properties of tetrahedral amorphous carbon from first principles", Appl. Phys. Lett. **75**, 644 (1999).

16. R. Lazzari, N. Vast, J.M. Besson, S. Baroni, and A. Dal Corso, "Atomic structure and vibrational properties of icosahedral B_4C boron carbide", Phys. Rev. Lett. **83**, 3230 (1999).

17. F. Favot and A. Dal Corso, "Phonon dispersions: Performance of the generalized gradient approximation", Phys. Rev. B. **60**, 11427 (1999).

18. V. Musolino, A. Dal Corso, and A. Selloni, "Initial stages of growth of copper on MgO(100): A first principles study", Phys. Rev. Lett. **83**, 2761 (1999).

19. M. Magagnini, P. Giannozzi, and A. Dal Corso, "Microscopic structure of the substitutional Aluminum defect in α-quartz", Phys. Rev. B **61**, 2621 (2000).

20. A. Dal Corso and S. de Gironcoli, "*Ab-initio* phonon dispersions of Fe and Ni", Phys. Rev. B **62**, 273 (2000).

21. F. Favot, A. Dal Corso and A. Baldereschi, "Adsorption geometry of benzene on Pd(110): Results of first-principles calculations", Europhys. Lett. **52**, 698 (2000).

22. S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Giannozzi "Phonons and related crystal properties from density-functional perturbation theory", Rev. Mod. Phys. **73**, 515 (2001).

23. F. Favot, A. Dal Corso and A. Baldereschi, "CO adsorbed on Cu(001): A comparison between local density approximation and Perdew, Burke, and Ernzerhof generalized gradient approximation" Jour. of Chem. Phys. **114**, 483 (2001).

24. F. Favot, A. Dal Corso and A. Baldereschi, "*Ab-initio* study of CO adsorption on Ni(110): effects on surface magnetism at low coverage", Phys. Rev. B **63**, 115416 (2001).

25. E. Tosatti, S. Prestipino, S. Koestlmeier, A. Dal Corso, and F. Di Tolla, "String tension and stability of magic tip-suspended nanowires", Science **291**, 288 (2001).

26. P. Umari, A. Pasquarello and A. Dal Corso, "Raman scattering intensities in α-quartz: A first-principles investigation", Phys. Rev. B **63**, 094305 (2001).

27. L. Savio, L. Vattuone, M. Rocca, V. De Renzi, S. Gardonio, C. Mariani, U. del Pennino, G. Cipriani, A. Dal Corso, S. Baroni "Substrate reconstruction and electronic surface states: Ag(001)", Surf. Sci. **486**, 65 (2001).

28. N. Manini, A. Dal Corso, M. Fabrizio, and E. Tosatti, "Electron–vibration coupling constants in positively charged fullerene", Philos. Mag. B **73**, 793 (2001).

29. A. Dal Corso "Density-functional perturbation theory with ultrasoft pseudopotentials", Phys. Rev. B **64**, 235118 (2001).

30. G. Cipriani, D. Loffreda, A. Dal Corso, S. de Gironcoli, and S. Baroni, "Adsorption of atomic oxygen on Ag(001): a study based on density-functional theory", Surf. Sci. **501**, 182 (2002).

31. N. Manini, G. Santoro, A. Dal Corso, E. Tosatti, "Sensitivity of the Mott transition to noncubic splitting of the orbital degeneracy: application to $NH_3K_3C_{60}$", Phys. Rev. B **66**, 115107 (2002).

32. A. Kokalj, A. Dal Corso, S. de Gironcoli, and S. Baroni, "The interaction of ethylene with perfect and defective Ag(001) surfaces", Jour. Phys. Chem. B **106**, 9839 (2002).

33. M. Lüders, A. Bordoni, N. Manini, A. Dal Corso, M. Fabrizio, and E. Tosatti, "Coulomb couplings in positively charged fullerene", Philos. Mag. B **82**, 1611 (2002).

34. M. Cococcioni, A. Dal Corso, and S. de Gironcoli, "Structural, electronic, and magnetic properties of Fe_2SiO_4, Fayalite: Comparison of LDA and GGA results", Phys. Rev. B **67**, 094106 (2003).

35. C. Bungaro, K.M. Rabe, and A. Dal Corso, "First-principles study of lattice instabilities in the ferromagnetic martensite Ni_2MnGa", Phys. Rev. B **68**, 134104 (2003).

36. F. Picaud, A. Smogunov, A. Dal Corso, and E. Tosatti, "Complex band structures and decay length in polyethylene chains", J. Phys.: Cond. Mat. **15**, 3731 (2003).

37. D. Loffreda, A. Dal Corso, S. Baroni, L. Savio, L. Vattuone, and M. Rocca, "Oxygen vibrations in O-Ag(001)", Surf. Sci. **530**, 26 (2003).

38. N. Bonini, A. Kokalj, A. Dal Corso, S. de Gironcoli, and S. Baroni, "Structure and dynamics of Oxygen adsorbed on Ag(100) vicinal surfaces", Phys. Rev. B **69**, 195401 (2004).

39. J. Tóbik and A. Dal Corso, "Electric fields with ultrasoft pseudo-potentials: applications to benzene and anthracene", Jour. of Chem. Phys. **120**, 9934 (2004).

40. A. Smogunov, A. Dal Corso, and E. Tosatti, "Ballistic conductance of magnetic Co and Ni nanowires with ultrasoft pseudo-potentials", Phys. Rev. B **70**, 045417 (2004).

41. A. Dal Corso and A. Mosca Conte, "Spin-orbit coupling with ultra-soft pseudopotentials: applications to Au and Pt", Phys. Rev. B **71**, 115106 (2005).

42. C. Grazioli, D. Alfè, S.R. Krishnakumar, S.S. Gupta, M. Veronese, S. Turchini, N. Bonini, A. Dal Corso, D.D. Sarma, S. Baroni, and C. Carbone, "Spin-flop ordering from frustrated ferro- and antiferromagnetic interactions: a combined theoretical and experimental study of a Mn/Fe(100) monolayer", Phys. Rev. Lett. **95**, 117201 (2005).

43. A. Kokalj, A. Dal Corso, S. de Gironcoli, and S. Baroni, "DFT study of a weakly π-bonded C_2H_4 on oxygen-covered Ag(100)", J. Phys. Chem. B **110**, 367 (2006).

44. A. Smogunov, A. Dal Corso, and E. Tosatti, "Ballistic conductance and magnetism in short tip-suspended Ni nanowires", Phys. Rev. B **73**, 075418 (2006).

45. A. Dal Corso, A. Smogunov, and E. Tosatti, "Ab initio ballistic conductance with spin-orbit coupling: application to monatomic wires", Phys. Rev. B **74**, 045429 (2006).

46. N. Bonini, A. Kokalj, A. Dal Corso, S. de Gironcoli, and S. Baroni, "Structure and dynamics of the missing-row reconstruction on O/Cu(001) and O/Ag(001)", Surf. Sci. **600**, 5074 (2006).

47. A. Dal Corso, "Density functional perturbation theory for lattice dynamics with fully relativistic ultrasoft pseudopotentials: application to fcc-Pt and fcc-Au", Phys. Rev. B **76**, 054308 (2007).

48. A. Smogunov, A. Dal Corso, A. Delin, R. Weht, and E. Tosatti, "Colossal magnetic anisotropy of monatomic free and deposited platinum nanowires", Nature Nanotechnology **3**, 22 (2008).

49. R. Mazzarello, A. Dal Corso, and E. Tosatti, "Spin-orbit modifications and splittings of deep surface states on clean Au(111)", Surf. Sci. **602**, 893 (2008).

50. N. Stojić, A. Dal Corso, B. Zhou, and S. Baroni, "Ab-initio simulation of photoemission spectroscopy in solids: plane-waves pseudopotential approach with applications to normal emission spectra of Cu(001) and Cu(111)", Phys. Rev. B **77**, 195116 (2008).

51. G. Sclauzero, A. Dal Corso, A. Smogunov, and E. Tosatti, "Interaction of a CO molecule with a Pt monatomic wire: electronic structure and ballistic conductance", Phys. Rev. B **78**, 085421 (2008).

52. A. Smogunov, A. Dal Corso, and E. Tosatti, "Magnetic phenomena, spin-orbit effects, and Landauer conductance in Pt nanowire contacts: Density-functional theory calculations", Phys. Rev. B **78**, 014423 (2008).

53. A. Dal Corso, "Ab-initio phonon dispersions of face centered cubic Pb: effects of spin-orbit coupling", J. Phys.: Condens. Matter **20**, 445202 (2008).

54. Y. Miura, R. Mazzarello, A. Dal Corso, A. Smogunov, and E. Tosatti, "Monatomic Au wire with a magnetic Ni impurity: electronic structure and ballistic conductance", Phys. Rev. B **78**, 205412 (2008).

55. P. Giannozzi, et al., "Quantum ESPRESSO: a modular and open-source software project for quantum simulations of materials", J. Phys.: Condens. Matter **21**, 395502 (2009).

56. A. Dal Corso, "Density functional perturbation theory within the projector augmented wave method", Phys. Rev. B **81**, 075123 (2010).

57. P. Gava, A. Dal Corso, A. Smogunov, and E. Tosatti, "Magnetism-induced ballistic conductance changes in Palladium nanocontacts", Eur. Phys. J. B **75**, 57 (2010).

58. A. Dal Corso, "Projector augmented-wave method: application to relativistic spin-density functional theory", Phys. Rev. B **82**, 075116 (2010).

59. S. Sorella, M. Casula, L. Spanu, and A. Dal Corso, "Ab-initio calculations for the β-tin diamond transition in Silicon: comparing theories with experiments", Phys. Rev. B **83**, 075119 (2011).

60. A. A. Adllan and A. Dal Corso, "Ultrasoft pseudopotentials and projector augmented-wave data sets: application to diatomic molecules", J. Phys.: Condens. Matter **23**, 425501 (2011).

61. G. Sclauzero, A. Dal Corso, and A. Smogunov, "Effect of stretching on the ballistic conductance of Au nanocontacts in presence of CO: a density functional study", Phys. Rev. B **85**, 165412 (2012).

62. G. Sclauzero, A. Dal Corso, and A. Smogunov, "Interaction of CO with an Au monatomic chain at different strains: electronic structure and ballistic transport", Phys. Rev. B **85**, 165411 (2012).

63. A. Dal Corso, "Projector augmented-wave method with spin-orbit coupling: applications to simple solids and zincblende-type semiconductors", Phys. Rev. B **86**, 085135 (2012).

64. G. Sclauzero and A. Dal Corso, "Efficient DFT+U calculations of ballistic electron transport: Application to Au monatomic chains with a CO impurity", Phys. Rev. B **87**, 085108 (2013).

65. A. Dal Corso, "Ab-initio phonon dispersions of transition and noble metals: effects of the exchange and correlation functional", J. Phys.: Condens. Matter **25**, 145401 (2013).

66. M. Palumbo, S.G. Fries, A. Dal Corso, F. Kormann, T. Hickel, and J. Neugebauer, "Reliability evaluation of thermophysical properties from first-principles calculations", J. Phys.: Condens. Matter **26**, 335401 (2014).

67. A. Dal Corso, "Pseudopotentials periodic table: from H to Pu", Computational Material Science **95**, 337 (2014).

68. A. Dal Corso, "Clean Ir(111) and Pt(111) electronic surface states: a first-principle fully relativistic investigation", Surf. Sci. **637-638**, 106 (2015).

69. K. Lejaeghere, et. al. "Reproducibility in density-functional theory calculations of solids", Science **351**, aad3000 (2016).

70. A. Dal Corso, "Elastic constants of Beryllium: a first-principles investigation", J. Phys.: Condens. Matter **28**, 075401 (2016).

71. M. Palumbo and A. Dal Corso, "Lattice dynamics and thermophysical properties of h.c.p. Os and Ru from the quasi-harmonic approximation", J. Phys.: Condens. Matter **29**, 395401 (2017).

72. M. Palumbo and A. Dal Corso, "Lattice dynamics and thermophysical properties of h.c.p. Re and Tc from the quasi-harmonic approximation", Phys. Status Solidi B: Basic Solid State Physics, **254**, 1700101 (2017).

73. P. Giannozzi, et. al., "Advanced capabilities for materials modelling with Quantum ESPRESSO" J. Phys.: Condens. Matter **29**, 465901 (2017).

74. A. Urru and A. Dal Corso, "Clean Os(0001) electronic surface states: a first-principle fully relativistic investigation", Surf. Sci. **671**, 17 (2018).

75. A. Urru and A. Dal Corso, "Spin-polarized electronic surface states of Re(0001): an ab-initio investigation", Surf. Sci. **686**, 22 (2019).

76. C. Malica and A. Dal Corso, "Temperature dependent atomic B-factor: an ab-initio calculation", Acta Cryst. A **75**, 624 (2019).

77. A. Urru and A. Dal Corso, "Density functional perturbation theory for lattice dynamics with fully relativistic ultrasoft pseudopotentials: The magnetic case", Phys. Rev. B **100**, 045115 (2019).

78. C. Malica and A. Dal Corso, "Quasi-harmonic temperature dependent elastic constants: Applications to Silicon, Aluminum, and Silver", J. of Phys.: Condens. Matter **32**, 315902 (2020).

79. C. Malica and A. Dal Corso, "Temperature dependent elastic constants and thermodynamic properties of BAs: an ab-initio investigation", Jour. of Applied Phys. **127**, 245103 (2020).

80. O. Motornyi, N. Vast, I. Timrov, O. Baseggio, S. Baroni, and A. Dal Corso, "Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method", Phys. Rev. B **102**, 035156 (2020).

81. A. Urru and A. Dal Corso, "Lattice dynamics effects on the magnetocrystalline anisotropy energy: application to MnBi", Phys. Rev. B **102**, 115126 (2020).

Conference proceedings, reply, errata

82. A. Dal Corso and A.C. Levi, "Zener Tunneling in the Amirav – Cardillo effect", Il Vuoto **21**, 218 (1992).

83. A. Dal Corso and A. Baldereschi, "*Ab-initio* study of the structural and electronic properties of adsorbates: CO on Cu(001)", Surface Review and Letters **4**, 885 (1997).

84. C. Massobrio, A. Pasquarello, and A. Dal Corso, "A first principle study of small Cu_n clusters based on local density and generalized-gradient approximations to density functional theory" Computational Material Science 10, 463 (1998). Proceedings of the Simposium "Computational Issues in Material Science", EMRS, June 1997, Strasbourg.

85. A. Dal Corso, A. Baldereschi, "Ab-Initio study of the vibrational properties of adsorbates: CO on Cu(001)" Proceedings of the VII Italian-Swiss workshop on Computational Condensed Matter Physics. 1997, Cagliari.

86. F. Favot, A. Dal Corso, and A. Baldereschi, "*Ab-initio* study of the $c(4 \times 2)$−benzene structure on Pd(110)", Proceedings of the Sixth International Conference on the Structure of Surfaces. 26 – 30 July, 1999, Vancouver, Canada. Surface Review and Letters, **6**, 903 (1999).

87. F. Di Tolla, A. Dal Corso, J. A. Torres, and E. Tosatti, "Electronic properties of ultra-thin Aluminum nanowires". Paper presented at the 18th European Conference on Surface Science 21 – 24 September 1999, Vienna, Austria. Surface Science **454-456**, 947 (2000).

88. N. Vast, J. Besson, S. Baroni, and A. Dal Corso, "Atomic structure and vibrational properties of icosahedral alpha-boron and B_4C boron carbide" Computational Material Science **17**, 127-132 (2000).

89. J.A. Torres, E. Tosatti, A. Dal Corso, F. Ercolessi, J.J. Kohanoff, F. Di Tolla, and J.M. Soler, Reply to "The puzzling stability of monoatomic gold wire is the result of small fluctuations" Surface Science **463**, 213 (2000).

90. A. Kokalj, A. Dal Corso, S. de Gironcoli, and S. Baroni, "Adsorption of ethylene on the Ag(001) surface" Surf. Sci. **507-510**, 62 (2002).

91. A. Smogunov, A. Dal Corso, and E. Tosatti, "Selective d-state conduction blocking in nickel nanocontacts" Surf. Sci. **507-510**, 609 (2002).

92. A. Smogunov, A. Dal Corso, and E. Tosatti, "Complex band structure with ultrasoft pseudopotentials: fcc Ni and Ni nanowire", Surf. Sci. **532-535**, 549 (2003).

93. F. Picaud, A. Dal Corso, and E. Tosatti, "Phonons softening in tip-stretched monatomic nanowires", Surf. Sci. **532-535**, 544 (2003).

94. A. Kokalj, A. Dal Corso, S. de Gironcoli, and S. Baroni, "Co-adsorption of ethylene and oxygen on the Ag(001) surface", Surf. Sci. **532-535**, 191 (2003).

95. A. Kokalj, A. Dal Corso, S. de Gironcoli, and S. Baroni, "Adsorption of ethylene on stepped Ag(n10) surfaces", Surf. Sci. **566-568**, 1018 (2004).

96. J. Tóbik, A. Dal Corso, S. Scandolo, and E. Tosatti, "Organic molecular crystals in electric fields", Surf. Sci. **566-568**, 644 (2004).

97. A. Smogunov, A. Dal Corso, and E. Tosatti, "Ballistic conductance of Ni nanowire with a magnetization reversal", Surf. Sci. **566-568**, 390 (2004).

98. N. Bonini, A. Kokalj, A. Dal Corso, S. de Gironcoli, and S. Baroni, "On-surface and subsurface adsorption of oxygen on stepped Ag(210) and Ag(410) surfaces", Surf. Sci. **566-568**, 1107 (2004).

99. N. Bonini, A. Dal Corso, A. Kokalj, S. de Gironcoli, and S. Baroni, "On-surface and sub-surface oxygen adsorption on Ag(210): vibrational properties", Surf. Sci. **587**, 50 (2005).

100. A. Aravindh, *et al.*, "$Si_x\ C_{1-x}\ O_2$ alloys: a possible route to stabilize carbon-based silica-like solids", Solid State Comm. **144**, 273 (2007).

101. G. Sclauzero, A. Dal Corso, A. Smogunov, and E. Tosatti, "Interaction of a CO molecule with a Pt monatomic chain: the top geometry", AIP Conf. Proc. **1018**, 201 (2008).

102. R. di Meo, A. Dal Corso, P. Giannozzi, and S. Cozzini, "Calculation of phonon dispersions on the GRID using Quantum ESPRESSO", ICTP lecture notes **24**, 163 (2009).

103. A. Dal Corso and L. Paulatto, "Density functional perturbation theory within the projector augmented-wave method: a few benchmarks for molecules and solids", AIP Conf. Proc. **1504**, 932 (2012).

104. O. Motornyi, M. Raynaud, A. Dal Corso, and N. Vast, Simulation of electron energy loss spectra with the `turboEELS` and `thermo_pw` codes, J. Phys.: Conf. Ser. **1136**, 012008 (2018).

Books chapters

105. A. Dal Corso "Reciprocal space integration and special points", in "Quantum-Mechanical *Ab-initio* calculation of the Properties of Crystalline Materials", Lecture Notes in Chemistry **67**, C. Pisani (Ed.) (1996, Springer, Berlin).

106. A. Dal Corso "A Pseudopotential Plane Waves Program (`PWscf`) and some Case Studies", in "Quantum-Mechanical *Ab-initio* calculation of the Properties of Crystalline Materials", Lecture Notes in Chemistry **67**, C. Pisani (Ed.) (1996, Springer, Berlin).

INVITED TALKS

Invited talks at international workshops or conferences

1. V Italian-Swiss workshop on computational condensed matter physics. 8 – 13 September, 1994. S. Margherita di Pula, Cagliari (Italy).
2. International workshop on computational condensed matter physics based on the electronic structure. 11 – 15 January, 1995. Trieste (Italy).
3. 1995 March meeting of the american physical society. 19 – 24 March, 1995. San Jose, California (United States).
4. Cecam workshop: First principle theory of polarization, fields and currents in insulators. 10 – 13 July, 1995. Lyon (France).
5. Cecam workshop: *Ab-initio* phonons. 1 – 3 July, 1996. Lyon (France).
6. Eighth international workshop on computational condensed matter physics: Total energy and force methods. 9 – 11 January, 1997. Trieste (Italy).
7. Cecam workshop: First-principle theory of ferroelectric materials. 3 – 5 July, 1997. Lyon (France).
8. VII Italian-Swiss workshop on computational condensed matter physics. 19 – 23 September, 1997. S. Margherita di Pula, Cagliari (Italy).
9. INFM meeting. 19 – 23 June, 1998. Rimini (Italy).
10. Cecam workshop: Electronic response functions in atoms, molecules, and solids. 5 – 7 October, 1998. Lyon (France).
11. Cecam workshop: Recent developments in the theory of Wannier functions and other localized electronic wavefunctions. 16 – 18 June, 1999. Lyon (France).
12. XIX Convegno di fisica teorica e struttura della materia, Fai della Paganella 2000. 26 – 29 March, 2000. Trento (Italy).
13. Cecam workshop: "Position operator **r** in extended systems within DFT and HF" September 29th – October 1st, 2003. Lyon (France).
14. Cecam workshop: "The anomalous Hall effect: Recent advances via the geometric-phase approach" 4 – 6 July, 2005. Lyon (France).
15. Italian-Swiss workshop on high-performance computing in materials science: "Modeling Materials at the Nano-Scale" 23 – 26 September, 2006. Palau (Sassari, Italy).
16. VII International conference of computational methods in sciences and engineering ICCMSE09, September 30th – October 4th, 2009. Rhodes (Crete, Greece).
17. Réunion générale GDR CoDFT, 27 – 30 June, 2011. Obernai (France).
18. Cecam workshop: "Topological insulators and non-perturbative spin-orbit coupling" 9 – 11 January, 2012. Lausanne (Switzerland).

Invited seminars or lectures

19. Scuola normale superiore, invited seminar. June 2nd, 1994. Pisa (Italy).
20. IV Scuola di chimica computazionale. "Calcolo quanto-meccanico di proprietà chimico fisiche dei materiali cristallini". 19 – 24 September, 1994. Torino (Italy).
21. Network school: "Hartree-Fock theory of the electronic structure of solids". 17 – 27 September, 1995. Torino (Italy).
22. Scuola nazionale di fisica della materia. 8 – 20 September, 1996. Torino (Italy).
23. Max-Plank-Institut für Festkörperforschung, invited seminar in Prof. M. Cardona group. October 18th, 1996. Stuttgart (Germany).
24. University of Neuchâtel: invited seminar in Prof. H. Beck group. May 27th, 1997. Neuchâtel (Switzerland).
25. Università di Torino: invited seminar in Prof. Pisani group. August 5th, 1997. Torino (Italy).
26. ICTP course on: "Calculation of material properties using total energy and force methods and *ab-initio* molecular dynamics". 9 – 18 August, 1999. Trieste (Italy).
27. ICTP Spring college: "Numerical methods in electronic structure theory". 7 – 25 May, 2001. Trieste (Italy).
28. ICTP Winter College: "Numerical methods in electronic structure theory". January 16 – February 4, 2003. Trieste (Italy).
29. IRRMA, EPFL (Lausanne) : invited seminar in Prof. Pasquarello group. October 18th, 2004. Lausanne (Switzerland).
30. Tutorial on: "*Ab-initio* simulation of the electronic, structural and dynamical properties of materials: a hands-on introduction to the `Quantum ESPRESSO` package (`PWscf-CP`)", 17 – 21 January 2005, ICTP, Trieste (Italy).
31. Tutorial on: "*Ab-initio* simulation of the electronic, structural and dynamical properties of materials: a hands-on introduction to the `Quantum ESPRESSO` package (`PWscf-CP`)", 26 – 30 September 2005, INFM-SLACS, Cagliari (Italy).
32. Bangalore summer school on "Electronic structure methods and their applications" in conjunction with conference on computational materials theory, 19 – 23 July 2006, Bangalore (India).
33. Tutorial on the `Quantum ESPRESSO` package after the "International symposium on multiscale modeling and simulation of materials", 7 – 11 July 2008, Fudan University, Shanghai (China).
34. Summer school on materials modeling from first principles: theory and practice, ICMR, University of California at Santa Barbara, 19 – 31 July, 2009. Santa Barbara (US).
35. Theory and practical use of `Quantum ESPRESSO`, Tyndall National Institute, Cork, 14 – 18 June, 2010. Cork (Ireland).
36. Summer school on atomistic simulations, SISSA, 5 – 23 July, 2010. Trieste (Italy).

37. Summer school on atomistic simulation techniques, SISSA, 11 – 30 July, 2011. Trieste (Italy).

38. Summer school on atomistic simulation techniques, SISSA, 9 – 27 July, 2012. Trieste (Italy).

39. Quantum ESPRESSO Developer Training, ICTP, 25 – 28 March, 2013. Trieste (Italy).

40. Summer school on atomistic simulation techniques, SISSA, 8 – 26 July, 2013. Trieste (Italy).

41. Summer school on atomistic simulation techniques, SISSA, 30 June – 18 July, 2014. Trieste (Italy).

42. Summer school on atomistic simulation techniques, SISSA, 6 – 24 July, 2015. Trieste (Italy).

43. Advanced Quantum ESPRESSO developers meeting: linear response, ICTP, 18 – 21 January 2016. Trieste (Italy).

44. Advanced workshop on high-performance high-throughput materials simulations using Quantum ESPRESSO, ICTP, 19 January, 2017. Trieste (Italy).

45. Summer school on atomistic simulation techniques, SISSA, 14 – 30 June, 2017. Trieste (Italy).

DIDACTIC ACTIVITY

- Electronic structure course at SISSA. 1999 – 2018, Trieste (Italy).
  Several Lectures on: Pseudopotential theory; Atomic calculations; Relativistic effects and spin-orbit coupling.
- Advanced Electronic structure course at SISSA. February - March 2019, Trieste (Italy).
  Several Lectures on: Introduction to crystallography; Density functional perturbation theory; Vibrational thermodynamics; Relativistic effects and spin-orbit coupling (36 hours).
- Course on "Advanced Electronic structure". Topical course for the SISSA PhD students, March 2018. (Density functional perturbation theory)
- Course on: "Numerical methods in electronic structure" for the "laurea specialistica" in computational physics of Udine University, (48 hours) April 18th – June 10th, 2005.
- Course on: "Electronic and phononic band structures" for the "laurea specialistica" in physics of Trento University, (18 hours) April 20th – May 30th, 2020.
- Course on: "Advanced topics in theoretical and computational physics" for the "laurea specialistica" in physics of Trento University, (10 hours) 13 – 21 April, 2011; (12 hours) April 26th – May 4th, 2012.
- Course on: "Elements of electronic structure of solids" for the "laurea specialistica" in physics of Trento University, (13 hours) 13 – 23 May, 2013; (16 hours) 19 – 29 May, 2014.
- Course on "Relativistic and scalar relativistic pseudopotential theory". Topical course for the SISSA PhD students (15 hours), February 27th – March 29th, 2012; March 11th - April 23rd, 2013; (22 hours) April - May 2016, 2017, 2018, 2019. June 02th-July 15th, 2020.
- Course on "Electronic structure II". Topical course for the SISSA PhD students (16 hours), February 18th – March 18th, 2014. (Pseudopotential theory and relativistic effects).
- Course on "Introduction to group theory for molecules and solids". Topical course for the SISSA PhD students (16 hours), June 6th – July 27th, 2016; June 2017.
- IV Scuola di chimica computazionale: "Calcolo quanto meccanico di proprietà chimico fisiche dei materiali cristallini". 19 – 24 September, 1994. Torino (Italy).
  Three lectures: Analysis of a plane wave density functional program for crystals; Reciprocal space integration and special points techniques; The `PWscf` code: application to silicon, aluminum and NaCl.
- Network School: "Hartree-Fock theory of the electronic structure of solids". 17 – 27 September, 1995. Torino (Italy).
  Two lectures: Density functional theory with plane waves; Linear response theory.
- Scuola nazionale di fisica della materia. 8 – 20 September, 1996. Torino (Italy).
  Two lectures+exercises: Analysis of a plane wave density functional program for crystals; Reciprocal space integration and special points techniques.
- ICTP course on: "Calculation of material properties using total energy and force methods and *ab-initio* molecular dynamics". 9 – 18 August, 1999. Trieste (Italy).
  One lecture: Berry phase and polarization theory.

- ICTP Spring college: "Numerical methods in electronic structure theory". 7 – 25 May, 2001. Trieste (Italy). Coorganizer with S. Baroni and S. de Gironcoli.
- ICTP Winter College: "Numerical methods in electronic structure theory". January 16th – February 4th, 2003. Trieste (Italy). Coorganizer with S. Baroni, S. de Gironcoli and P. Giannozzi.
- Tutorial on: "*Ab-initio* simulation of the electronic, structural and dynamical properties of materials: a hands-on introduction to the `Quantum ESPRESSO` package (`PWscf-CP`)", 17 – 21 January 2005, ICTP, Trieste (Italy). Coorganizer with S. de Gironcoli, S. Baroni, and S. Scandolo.
- Tutorial on: "*Ab-initio* simulation of the electronic, structural and dynamical properties of materials: a hands-on introduction to the `Quantum ESPRESSO` package (`PWscf-CP`)", 26 – 30 September 2005, INFM-SLACS, Cagliari (Italy).
  Two lectures: Density functional perturbation theory; Ballistic conductance.
- Bangalore summer school on: "Electronic structure methods and their applications" in conjunction with conference on computational materials Theory, 19 – 23 July 2006, Bangalore (India).
- Tutorial on the `Quantum ESPRESSO` package after the "International symposium on multi-scale modeling and simulation of materials", 7 – 11 July 2008, Fudan University, Shanghai (China).
- Summer school on: "Materials modeling from first principles: theory and practice", ICMR, University of California at Santa Barbara, 19 – 31 July, 2009. Santa Barbara (US).
- Tutorial on: "Theory and practical use of `Quantum ESPRESSO`", Tyndall National Institute, Cork, 14 – 18 June, 2010. Cork (Ireland).
- Summer school on atomistic simulations, SISSA, 5 – 23 July, 2010. Trieste (Italy).
- Summer school on atomistic simulation techniques, SISSA, 11 – 30 July, 2011. Trieste (Italy).
- Summer school on atomistic simulation techniques, SISSA, 9 – 27 July, 2012. Trieste (Italy).
- "Quantum ESPRESSO Developer Training", ICTP, 25 – 28 March, 2013. Trieste (Italy).
- Summer school on atomistic simulation techniques, SISSA, 8 – 26 July, 2013. Trieste (Italy).
- Summer school on atomistic simulation techniques, SISSA, 30 June – 18 July, 2014. Trieste (Italy).
- Summer school on atomistic simulation techniques, SISSA, 6 –24 July, 2015. Trieste (Italy).
- Summer school on atomistic simulation techniques, SISSA, 14 –30 June, 2017. Trieste (Italy).
- Quantum ESPRESSO developer meeting, ICTP, 9 January, 2017. Trieste (Italy).
- Advanced workshop on high-performance high-throughput materials simulations using Quantum ESPRESSO, ICTP, 19 January, 2017. Trieste (Italy).

- Supervisor (with Prof. A. Baldereschi) of the Ph.D. thesis: "Electronic, structural and dielectric properties of solids with Wannier functions" by P. Fernández. 1994 – 1998, EPF-Lausanne.
- Supervisor (with Prof. A. Baldereschi) of the diploma thesis: "Thermodynamical properties of gold" by G. Inganni. 1997 – 1998, EPF-Lausanne.
- Supervisor (with Prof. A. Baldereschi) of the Ph.D. thesis: "Metallic surfaces with adsorbates" by F. Favot. 1997 – 2000, EPF-Lausanne.
- Supervisor (with Profs. S. Baroni and S. de Gironcoli) of the Ph.D. thesis: "*Ab-initio* study of oxygen adsorption on selected transition metal surfaces" by G. Cipriani. 1999 – 2000, SISSA (Trieste).
- Supervisor (with Profs. S. Baroni and S. de Gironcoli) of the Master thesis: "*Ab-initio* study of fayalite (Fe_2 Si O_4)" by M. Cococcioni. 2000, SISSA (Trieste).
- Supervisor (with Prof. E. Tosatti) of the "Tesi di laurea specialistica": "Ballistic conductance in palladium nanocontacts" by P. Gava. 2004, Pisa University.
- Supervisor of the "Tesi di laurea specialistica": "Studio da principi primi dell'interazione di una molecola di CO con un nanofilo monoatomico di Pt" by G. Sclauzero. 2006, Udine University.
- Supervisor of the Master thesis: "Electronic structure and ballistic conductance of a Pt monatomic wire interacting with a CO molecule: comparing selected geometries" by G. Sclauzero. 2007, SISSA (Trieste).
- Supervisor of the PhD thesis: "Modeling CO adsorption on Au and Pt monatomic chains and nanocontacts" by G. Sclauzero. April 2010, SISSA (Trieste).
- Supervisor of the Tirocinio work of F. Zadra (undergraduate student of Trieste University). October 2015 - January 2016.
- Supervisor of the Master work: "Clean Os(0001) electronic surface states: a first-principle fully relativistic investigation" by A. Urru. October 2017, SISSA (Trieste).
- Supervisor of the Master work: "Temperature dependent atomic B-factor: an ab-initio calculation" C. Malica. October 2018, SISSA (Trieste).
- Supervisor of the PhD work: "Lattice dynamics with Fully Relativistic Pseudopotentials for magnetic systems, with selected applications" A. Urru. November 2020, SISSA (Trieste).

CONFERENCES AND SCHOOLS ORGANIZATION

- CECAM workshop: "Recent developments in the theory of Wannier functions and other localized electronic wavefunctions". 16 – 18 June, 1999. Lyon (France). Coorganizer with R. Resta and D. Vanderbilt.
- ICTP Spring college: "Numerical methods in electronic structure theory". 7 – 25 May, 2001. Trieste (Italy). Coorganizer with S. Baroni and S. de Gironcoli.
- ICTP Winter College: "Numerical methods in electronic structure theory". January 16th – February 4th, 2003. Trieste (Italy). Coorganizer with S. Baroni, S. de Gironcoli and P. Giannozzi.
- Tutorial on: "*Ab-initio* simulation of the electronic, structural and dynamical properties of materials: a hands-on introduction to the `Quantum ESPRESSO` package (`PWscf-CP`)", 17 – 21 January 2005, ICTP, Trieste (Italy). Coorganizer with S. de Gironcoli, S. Baroni, and S. Scandolo.
- Local organizer of the:"XII international workshop on computational physics and materials science: Total energy and force methods" 13 – 15 January 2005 (Trieste). Coorganizer with G. Galli and E. Artacho.
- CECAM Summer school on atomistic simulation techniques, SISSA, 14 –30 June, 2017. Trieste (Italy). Coorganizer with S. de Gironcoli and A. Magistrato.

PARTICIPATION TO EXAM COMMITTEE

- SISSA entrance examination. Condensed matter sector (2000-2020). Trieste (Italy).
- Master exam of the SISSA condensed matter sector. October 2000-2020. Trieste (Italy).
- PhD exam of the SISSA condensed matter sector. October 2000-2020. Trieste (Italy).
- Fast-track to the PhD course entrance examination. SISSA Condensed matter sector (2016-2020). Trieste (Italy).
- PhD exam of F. Favot. December 13, 2000. EPF-Lausanne (Switzerland).
- Laurea specialistica exam of P. Gava. September 30th, 2004. Pisa (Italy).
- Laurea specialistica exam of G. Sclauzero. October 11th, 2006. Udine (Italy).
- PhD exam of L. Giacomazzi. January 22nd, 2007. EPF-Lausanne (Switzerland).
- Entrance examination to the XXV corso di dottorato in scienza dei materiali. Milano–Bicocca University. 3 – 5 November, 2009. Milan (Italy).
- Entrance examination to the XXVIII corso di dottorato in scienza dei materiali. Milano–Bicocca University. 5 – 7 November, 2012. Milan (Italy).
- PhD exam of A. Motornyi. December 21st, 2018. École Polytechnique, Université Paris Saclay (France).

REFEREE FOR INTERNATIONAL JOURNALS

- Physical Review Letters
- Physical Review B
- Journal of Physics: Condensed Matter
- Surface Science
- Applied Surface Science
- European Physical Journal - Applied Physics
- Journal of the American Ceramic Society
- International Journal of Modern Physics B
- npj Computational Materials
- Modern Physics Letters B
- Advances in Material Science

PRIZES AND AWARDS

- Outstanding Referee of the American Physical Society (2017).

RESEARCH FUNDS

- Project Manager for several projects on "*Ab-initio* simulation of metallic surfaces and nanostructures" (2002 – 2005) and "Spin-orbit effects on nanocontacts, nanowires, surfaces and bulk" (2006 – 2008) within the "Iniziativa trasversale calcolo parallelo" of INFM.
- MIUR – COFIN 2004. Local coordinator of the project: "Nanoattrito superficiale di solidi, punte, e liquidi: teoria, simulazione, ed esperimento".