Vincenzo Fiorentini

Publication List

(updated : Jan 2012)

A – Edited books [2] and Special Issues [3]

1. **V. Fiorentini** and F. Meloni (eds.), *Advances in Computational Materials Science* (Società Italiana di Fisica, Bologna 1997), 119 pages.

2. **V. Fiorentini** and F. Meloni (eds.), *Advances in Computational Materials Science – II* (Società Italiana di Fisica, Bologna 1998), 122 pages.

3. **V. Fiorentini**, F. Meloni, and P. Ruggerone, guest editors: *Computational Materials Science IX*, Comput. Mat. Sci. **20**, Nos. 3-4 (2001).

4. P. Ruggerone, **V. Fiorentini**, and F. Meloni, guest editors: *Computational Materials Science X*, Comput. Mat. Sci. **22**, Nos. 3-4 (2002).

5. P. Ruggerone, **V. Fiorentini**, and F. Meloni, guest editors: *Computational Materials Science*, Comput. Mat. Sci. **30**, Nos. 1-2 (2004).

B – Papers on peer-reviewed international journals [100]

1. **V. Fiorentini** and A. Baldereschi:
Interpretation of double acceptor spectra in Ge,
Solid State Commun. **69**, 953-958 (1989).

2. **V. Fiorentini**:
Self-consistent DFT calculations of electronic states in superlattices and quantum wells with arbitrary compositional and doping profiles,
Semicond. Sci. Technol. **5**, 211-217 (1990).

3. **V. Fiorentini**:
Semiconductor band structures at zero pressure,
Phys. Rev. B **46**, 2086-2091 (1992).

4. **V. Fiorentini** and A. Baldereschi:
Semiempirical self-energy correction to LDA bands of semiconductors, and a scaling law for the scissor operator,
J. Phys. Condensed Matter **4**, 5967-5976 (1992).

5. **V. Fiorentini**:
A note on ab-initio semiconductor band structures,
Solid State Commun. **81**, 871-875 (1992).

6. **V. Fiorentini**, M. Methfessel and M. Scheffler:
Electronic and structural properties of GaN by the full-potential LMTO method: the role of the d electrons,
Phys. Rev. B **47**, 13353-13362 (1993).

7. **V. Fiorentini**, M. Methfessel and M. Scheffler:
   Reconstruction mechanism of fcc transition-metal (001) surfaces,
   Phys. Rev. Lett. **71**, 1051-1054 (1993).

8. S. Oppo, **V. Fiorentini** and M. Scheffler:
   Theory of adsorption and surfactant effect of Sb on Ag (111),
   Phys. Rev. Lett. **71**, 2437-2440 (1993).

9. **V. Fiorentini**, S. Oppo, and M. Scheffler:
   Towards an understanding of surfactant action on the epitaxial growth of metals: the case of Sb on Ag (111),
   Appl. Phys. A **60**, 399-402 (1995).

10. **V. Fiorentini**:
    Effective-mass single and double acceptor spectra in GaAs,
    Phys. Rev. B **51**, 10161-10163 (1995)

11. **V. Fiorentini** and A. Baldereschi:
    Dielectric scaling of the self-energy scissor operator in semiconductors and insulators,
    Phys. Rev. B **51**, 17196-17198 (1995)

12. A. Bosin, **V. Fiorentini**, A. Lastri and G. B. Bachelet:
    Local norm-conserving pseudohamiltonians,
    Phys. Rev. A **52**, 236-257 (1995)

13. **V. Fiorentini** and M. Methfessel:
    Extracting convergent surface energies from slab calculations,
    J. Phys. Cond. Matter **8**, 6525-6529 (1996).

14. **V. Fiorentini**, D. Fois and S. Oppo:
    Inhibited Al diffusion and growth roughening of Ga-coated Al (100),
    Phys. Rev. Lett. **77**, 695-698 (1996).

15. A. Filippetti and **V. Fiorentini**:
    Reconstructions of Ir (100) and (110): an ab initio study,
    Surface Science **377**, 112-116 (1997).

16. F. Bernardini, **V. Fiorentini**, and A. Bosin:
    Theoretical evidence for efficient p-type doping of GaN using beryllium,
    Appl. Phys. Lett. **70**, 2990-2992 (1997).

17. C. M. Carbonaro, **V. Fiorentini**, and S. Massidda:
    Ab initio study of oxygen vacancies in α-quartz,
    J. Non-Cryst. Solids **221**, 89-96 (1997).

18. F. Bernardini, **V. Fiorentini**, and D. Vanderbilt:
    Spontaneous polarization and piezoelectric constants of III-V nitrides,
    Phys. Rev. B **56**, R10024-R10027 (1997).

19. F. Bernardini, **V. Fiorentini**, and D. Vanderbilt:
    Polarization-based calculation of the dielectric tensor of polar crystals,
    Phys. Rev. Lett. **79**, 3958-3961 (1997).

20. F. Bernardini and **V. Fiorentini**:
Macroscopic polarization and band offsets at nitride heterojunctions,
Phys. Rev. B **57**, R9427-R9430 (1998).

21. S. Oppo and **V. Fiorentini**:
No in-plane reconstruction of Cu (001),
Phys. Rev. Lett. **81**, 4278-4278 (1998).

22. F. Bernardini and **V. Fiorentini**:
Electronic dielectric constants of insulators by the polarization method,
Phys. Rev. B **58**, 15292-15295 (1998).

23. A. Filippetti, **V. Fiorentini**, G. Cappellini, and A. Bosin:
Ionicity and relaxation behavior at III-V nitride surfaces,
phys. stat. sol. (a) **170**, 265-268 (1998).

24. A. Fara, F. Bernardini, and **V. Fiorentini**:
Theoretical evidence for the semi-insulating character of AlN,
J. Appl. Phys. **85**, 2001-2003 (1999).

25. U. Hansen, P. Vogl, and **V. Fiorentini**:
Atomistic modelling of large-scale metal film growth fronts,
Phys. Rev. B **59**, R7856-R7859 (1999).

26. A. Filippetti, **V. Fiorentini**, G. Cappellini, and A. Bosin:
Anomalous relaxations and chemical trends at III-V nitride non-polar surfaces,
Phys. Rev. B **59**, 8026-8031 (1999).

27. F. Della Sala, A. Di Carlo, P. Lugli, F. Bernardini, **V. Fiorentini**, R. Scholz, and J.-M. Jancu:
Free-carrier screening of polarization fields in wurtzite GaN/InGaN laser structures,
Appl. Phys. Lett. **74**, 2002-2004 (1999).

28. U. Hansen, P. Vogl, and **V. Fiorentini**:
Quasi-harmonic vs. "exact" surface free energies of Al: a systematic study employing a new interatomic potential,
Phys. Rev. B **60**, 5055-5064 (1999).

29. **V. Fiorentini**, F. Bernardini, F. Della Sala, A. Di Carlo, and P. Lugli:
Effects of macroscopic-polarization built-in electrostatic fields in III-V nitrides multi-quantum-wells,
Phys. Rev. B **60**, 8849-8858 (1999).

30. A. Filippetti and **V. Fiorentini**:
Faceting and stress in the missing-row reconstructions of (110) transition-metal surfaces,
Phys. Rev. B **60**, 14366-14371 (1999).

31. F. Bernardini and **V. Fiorentini**:
Spontaneous vs. piezoelectric polarization in III-V nitrides: conceptual aspects and practical consequences,
phys. stat. sol. (b) **216**, 391-398 (1999).

32. M. Methfessel, **V. Fiorentini**, and S. Oppo:
Connection between charge transfer and alloying core-level shifts using density-functional calculations,
Phys. Rev. B **61**, 5229-5236 (2000).

33. A. Filippetti and **V. Fiorentini**:
Theory and applications of the stress density,
Phys. Rev. B **61**, 8433-8442 (2000).

34. F. Bernardini and **V. Fiorentini**:
Incorporation, diffusion, and electrical activity of Li in GaN,
Phys. Rev. B **61**, 12598-12601 (2000).

35. A. Di Carlo, F. Della Sala, P. Lugli, **V. Fiorentini**, and F. Bernardini:
Doping screening of polarization fields in nitride heterostructures,
Appl. Phys. Lett. **76**, 3950-3952 (2000).

36. F. Bernardini and **V. Fiorentini**:
Polarization fields in nitride nanostructures: ten points to think about,
Appl. Surf. Sci. **166**, 23-29 (2000).

37. F. Bernardini, M. Peressi, and **V. Fiorentini**:
Band offsets and stability of BeTe/ZnSe (100) heterojunctions,
Phys. Rev. B **62**, R16302-R16305 (2000).

38. A. Filippetti and **V. Fiorentini**:
Stress and reconstruction on (001) transition-metal surfaces,
Comput. Mater. Sci. **20**, 423-428 (2001).

39. C. M. Carbonaro, **V. Fiorentini**, and F. Bernardini:
Proof of the thermodynamical stability of the E' center in SiO_2,
Phys. Rev. Lett. **86**, 3064-3067 (2001).

40. F. Trudu, **V. Fiorentini**, P. Ruggerone, and U. Hansen:
Roughening of close packed singular surfaces,
Phys. Rev. B **63**, 153402-(1-4) (2001).

41. F. Bernardini, **V. Fiorentini**, and D. Vanderbilt:
Accurate calculation of polarization-related quantities in semiconductors,
Phys. Rev. B **63**, 193201–(1-4) (2001).

42. A. Zoroddu, F. Bernardini, P. Ruggerone, and **V. Fiorentini**:
First-principles prediction of structure, energetics, formation enthalpy, elastic constants, polarization, and piezoelectric constants of AlN, GaN, and InN: comparison of local and gradient-corrected density-functional theory,
Phys. Rev. B **64**, 045208–(1-6) (2001).

43. F. Bernardini and **V. Fiorentini**:
Non-linear macroscopic polarization in III-V nitride alloys,
Phys. Rev. B **64**, 085207–(1-7) (2001).

44. **V. Fiorentini**, F. Bernardini, and O. Ambacher:
Evidence for non-linear macroscopic polarization in III-V nitride alloy heterostructures,
Appl. Phys. Lett. **80**, 1204-1206 (2002).

45. O. Ambacher, J. Majewski, C. Miskys, A. Link, M. Hermann, M. Eickhoff, M. Stutzmann, F. Bernardini, **V. Fiorentini**, V. Tilak, B Shaff, and L. F. Eastman:
Pyroelectric properties of Al(In)GaN/GaN hetero- and quantum well structures,
J. Phys: Condens. Matter **14**, 3399-3434 (2002).

46. F. Bernardini and **V. Fiorentini**:
Nonlinear behavior of spontaneous and piezoelectric polarization in III-V nitride alloys,
phys. stat. sol. (a) **190**, 65-73 (2002)

47. P. Vogl, U. Hansen, and **V. Fiorentini**:
Multiscale approaches for metal thin film growth,
Comput. Mater. Sci. **24**, 58-65 (2002).

48. F. Bernardini and **V. Fiorentini**:
First-principles calculation of the piezoelectric tensor $\overleftrightarrow{d}$ *of III-V nitrides*,
Appl. Phys. Lett. **80**, 4145-4147 (2002).

49. C. M. Carbonaro, **V. Fiorentini**, and F. Bernardini:
Stability of Ge-related point defects and complexes in Ge-doped SiO_2,
Phys. Rev. B **66**, 233201-(1-4) (2002).

50. **V. Fiorentini** and G. Gulleri:
First-principles theoretical evaluation of crystalline zirconia and hafnia as gate oxides for Si microelectronics,
Phys. Rev. Lett. **89**, 266101–(1-4) (2002).

51. **V. Fiorentini**:
Origin of the efficient light emission at inversion domain boundaries in GaN,
Appl. Phys. Lett. **82**, 1182-1184 (2003).

52. M. Mura, P. Ruggerone, and **V. Fiorentini**:
Ordered vs disordered growth of copper quantum wires on Mo and W vicinal surfaces,
Phys. Rev. B **67**, 153406–(1-4) (2003).

53. O. Ambacher, M. Eickhoff, A. Link, M. Hermann, M. Stutzmann, F. Bernardini, **V. Fiorentini**, Y. Smorchkova, J. Speck, U. Mishra, W. Shaff, V. Tilak, and L. F. Eastman:
Electronics and sensors based on pyroelectric AlGaN/GaN heterostructures - Part A: Polarization and pyroelectronics,
phys. stat. sol. (c) **0**, 1878-1907 (2003).

54. G. M. Lopez and **V. Fiorentini**:
Vibrational modes of three-body self-interstitial clusters in silicon,
J. Phys.: Condensed Matter **15**, 7851-7858 (2003).

55. A. Polimeni, G. Baldassarri, F. Masia, A. Frova, M. Capizzi, S. Sanna, **V. Fiorentini**, P. J. Klar, and W. Stolz:
Tunable variation of the electron effective mass and exciton Bohr radius in hydrogenated GaAsN alloys,
Phys. Rev. B **69**, 041201(R) –(1-4) (2004).

56. P. Delugas and **V. Fiorentini**:
Energetics of transient enhanced diffusion of boron in Ge and SiGe,
Phys. Rev. B **69**, 085203-(1-5) (2004).

57. S. Sanna and **V. Fiorentini**:
Lattice constant, effective mass, and gap recovery in hydrogenated GaAsN,
Phys. Rev. B **69**, 125208-(1-6) (2004).

58. G. M. Lopez and **V. Fiorentini**:
Structure, stability, and extrinsic levels of small self-interstitials clusters in Si,
Phys. Rev. B **69**, 155206-(1-8) (2004).

59. A. Polimeni, G. Baldassarri, F. Masia, A. Frova, M. Capizzi, S. Sanna, **V. Fiorentini**, P. J. Klar, and W. Stolz:
Tuning of the electron effective mass and exciton wavefunction size in $GaAs_{1-x}N_x$,
Physica E **21**, 747-751 (2004).

60. L. Marsella and **V. Fiorentini**:
Structure and stability of rare-earth and transition-metal oxides,
Phys. Rev. B **69**, 172103-(1-4) (2004).

61. C. Melis, G. M. Lopez and **V. Fiorentini**:
Anomalous energetics and defect-assisted diffusion of Ga in silicon,
Appl. Phys. Lett. **85**, 4902-4904 (2004)

62. P. Schirra, G. M. Lopez and **V. Fiorentini**:
Complexes, clustering, and native-defect assisted diffusion of aluminum in silicon,
Phys. Rev. B **70**, 245201-(1-7) (2004).

63. E. Bonera, G. Scarel, M. Fanciulli, P. Delugas, and **V. Fiorentini**:
Dielectric properties of high-κ *oxides: theory and experiment for* Lu_2O_3,
Phys. Rev. Lett. **94**, 027602-(1-4)(2005).

64. G. Malloci, G. Mulas, G. Cappellini, **V. Fiorentini**, and I. Porceddu:
Theoretical electron affinities of PAHs and electronic absorption spectra of their mono-anions,
Astronomy&Astrophysics **432**, 585-594 (2005).

65. P. Delugas and **V. Fiorentini**:
Dielectric properties of two phases of lutetium oxide,
Microelectr. Reliabil. **45**, 831-833 (2005).

66. G. Ciatto, F. d'Acapito, F. Boscherini, S. Sanna, **V. Fiorentini**, A. Polimeni, M. Capizzi, P. J. Klar, W. Stolz, and S. Mobilio:
Comparison between experimental and theoretical determination of the local structure of the $GaAs_{1-y}N_y$ *dilute nitride alloy*,
Phys. Rev. B **71**, 115210-(1-8) (2005).

67. L. Romano, A. M. Piro, M. G. Grimaldi, G. M. Lopez, and **V. Fiorentini**:
Influence of point defects injection on the stability of supersaturated Ga-Si solid solution,
Phys. Rev. B **71**, 165201-(1-6) (2005).

68. P. Delugas, **V. Fiorentini**, and A. Filippetti:
Dielectric properties and long-wavelength optical modes of the high-κ *oxide* $LaAlO_3$,
Phys. Rev. B **71**, 134302 (2005).

69. A. Filippetti and **V. Fiorentini**:
Coexistence of ionic and metallic bonding in noble-metal oxides,
Phys. Rev. B **72**, 035128 (2005).

70. G. M. Lopez, **V. Fiorentini**, G. Impellizzeri, S. Mirabella, and E. Napolitani:
Fluorine in Si: native-defect complexes and suppression of impurity diffusion,
Phys. Rev. B **72**, 045219 (2005).

71. A. Filippetti and **V. Fiorentini**:
Magnetic ordering in CuO from first-principles : a cuprate antiferromagnet with fully three-dimensional exchange interactions,
Phys. Rev. Lett. **95**, 086405 (2005).

72. **V. Fiorentini** and G. M. Lopez:
Comment on Ab Initio Calculations to Model Anomalous Fluorine Behavior,
Phys. Rev. Lett. **96**, 039601 (2006).

73. G. M. Lopez and **V. Fiorentini**:
Large fluorine-vacancy clusters in Si and their capture efficiency for self-interstitials,
Appl. Phys. Lett. **89**, 092113 (2006).

74. A. Filippetti and **V. Fiorentini**:
Double-exchange driven ferromagnetic metal-paramagnetic insulator transition in Mn-doped CuO,
Phys. Rev. B **74**, 220401(R) (2006).

75. A. Filippetti and **V. Fiorentini**:
Self-interaction-free density-functional band theory for magnetic cuprates,
J. Magn. Magnetic Mat. **310**, 1648 (2007).

76. P. Delugas, **V. Fiorentini**, A. Filippetti, and G. Pourtois:
Cation charge anomalies and high-κ dielectric behavior in $DyScO_3$,
Phys. Rev. B **75**, 115126 (2007).

77. A. Filippetti and **V. Fiorentini**:
Magnetic ordering under strain and spin-Peierls dimerization in $GeCuO_3$,
Phys. Rev. Lett. **98**, 196403 (2007).

78. G. Colizzi, A. Filippetti, and **V. Fiorentini**:
Magnetism of $La_{0.625}Sr_{0.375}MnO_3$ under high-pressure from principles,
Phys. Rev. B **76**, 064428 (2007).

79. P. Delugas, **V. Fiorentini**, A. Filippetti, and G. Pourtois:
Conservation of dielectric constant upon amorphization in high-κ perovskite oxides,
Phys. Rev. B **76**, 104112 (2007).

80. K. Xiong, P. Delugas, J. C. Hooker, **V. Fiorentini**, J. Robertson, D. M. Liu, and G. Pourtois :
Te-induced modulation of the Mo/HfO_2 interface effective work function,
Appl. Phys. Lett. **92**, 113504 (2008).

81. P. Delugas, **V. Fiorentini**, and A. Filippetti:
Dielectric constant boost in amorphous sesquioxides,
Appl. Phys. Lett. **92**, 172903 (2008).

82. A. Filippetti and **V. Fiorentini**:
Metal-insulator transitions and singlet polarons in one-dimensional $Ca_{2+x}Y_{2-x}Cu_5O_{10}$,
Phys. Rev. B **77**, 235124 (2008).

83. A. Filippetti, G. M. Lopez, M. Mantega, and **V. Fiorentini**:
Chain metallicity and antiferro-paramagnetism competition in underdoped $YBa_2Cu_3O_{6+x}$: a first principles description,
Phys. Rev. B **78**, 233103 (2008)

84. G. Colizzi, A. Filippetti, F. Cossu, and **V. Fiorentini**:
Interplay of strain and magnetism in $La_{1-x}Sr_xMnO_3$ from first principles,
Phys. Rev. B **78**, 235122 (2008)

85. D. Puggioni, A. Filippetti, and **V. Fiorentini**:
Fermi-surface pockets in $YBa_2Cu_3O_{6.5}$: A comparison of ab initio techniques,
Phys. Rev. B **79**, 064519 (2009)

86. G. Colizzi, G. Biddau, and **V. Fiorentini**:
Indium on Cu (100) from first principles: energetics, complex formation and diffusion of adsorbates and vacancies on terraces and at steps,
Phys. Rev. B **79**, 165441 (2009)

87. G. Colizzi, A. Filippetti, F. Cossu, and **V. Fiorentini**:
Magnetic couplings vs. stress and strain in epitaxial (La,Sr)MnO_3,
Eur. Phys. J. B **70**, 343 (2009)

88. P. Delugas, **V. Fiorentini**, and A. Filippetti:
Dielectric and vibrational properties of bixbyite sesquioxides,
Phys. Rev. B **80**, 104301 (2009)

89. A. Filippetti and **V. Fiorentini**:
A practical first-principles band-theory approach to the study of correlated materials,
Eur. Phys. J. B **71**, 139 (2009)
free on-line at `http://www.epj.org/_pdf/HP_EPJB_practical_first-principles.pdf`

90. G. Peralta, D. Puggioni, A. Filippetti, and **V. Fiorentini**:
Jahn-Teller stabilization of magnetic and orbital ordering in rocksalt CuO,
Phys. Rev. B **80**, 140408(R) (2009)

91. A. Filippetti, D. Puggioni, and **V. Fiorentini**:
Fermi-surface pockets in magnetic underdoped cuprates from first principles,
Europhys. Lett. **88**, 67009 (2009)

92. P. Delugas, P. Alippi, **V. Fiorentini**, and V. Raineri:
Reorientable dipolar Cu_{Ca} anti-site and anomalous screening in $CaCu_3Ti_4O_{12}$,
Phys. Rev. B **81**, 081104(R) (2010)

93. M. Cantoni, D. Petti, S. Brivio, R. Bertacco, I. Pallecchi, D. Marré, G. Colizzi, A. Filippetti, and **V. Fiorentini**:
Band alignment at the $Cu_2O/La_{0.67}Sr_{0.33}MnO_3$ interfaces: a combined experimental-theoretical determination,
Appl. Phys. Lett. **97**, 032115 (2010)

94. G. Colizzi, A. Filippetti, and **V. Fiorentini**:
Multiferroicity and orbital ordering in $Pr_{0.5}Ca_{0.5}MnO_3$ from first principles,
Phys. Rev. B **82**, 140101(R) (2010)

95. G. M. Lopez, A. Filippetti, M. Mantega, and **V. Fiorentini**:
First-principles calculation of electronic and structural properties of $YBa_2Cu_3O_{6+y}$,
Phys. Rev. B **82**, 195122 (2010)

96. P. Delugas, A. Filippetti, **V. Fiorentini**, D. I. Bilc, D. Fontaine, and P. Ghosez:
Spontaneous 2-dimensional carrier confinement at the n-type SrTiO3/LaAlO3 interface,
Phys. Rev. Lett. **106**, 166807 (2011)

97. P. Alippi, F. Filippone, A. Amore Bonapasta, and **V. Fiorentini**:
Bound electron and hole states of the Fe impurity in wurtzite GaN from hybrid density-functional calculations,
Phys. Rev. B **84**, 033201 (2011)

98. T. Archer, S. Sanvito, C. Franchini, J. He, A. Filippetti, P. Delugas, D. Puggioni, **V. Fiorentini**, R. Tiwari, and P. Majumdar:
Exchange interactions and magnetic phases of transition metal oxides: Benchmarking advanced ab initio methods,
Phys. Rev. B **84**, 115114 (2011)

99. A. Filippetti, C. D. Pemmaraju, S. Sanvito, P. Delugas, D. Puggioni, and **V. Fiorentini**:
Variational pseudo-self-interaction-corrected density-functional approach to the ab-initio description of correlated solids and molecules,
Phys. Rev. B **84**, 195127 (2011)

100. P. Alippi and **V. Fiorentini**:
Magnetism and unusual Cu valency in quadruple perovskites
Eur. Phys. J. **85**, in print (2012)

*** Submitted**

101. A. Filippetti, P. Delugas, M. J. Verstraete, I. Pallecchi, A. Gadaleta, D. Marré, D. F. Li, S. Gariglio, and **V. Fiorentini**:
Thermopower in oxide heterostructures: the $SrTiO_3/LaAlO_3$ interface
Phys. Rev. Lett., submitted (2011)

102. P. Alippi, A. Filippetti, and **V. Fiorentini**:
Predictivity of advanced ab initio methods: the case of the gaps of $CaCu_3Ti_4O_{12}$
Phys. Rev. B, submitted (2012)

**** In preparation**

103. D. Puggioni, A. Filippetti, and **V. Fiorentini**:
Assessing charge disproportionation in multiple-valence oxides: the case of La_2NiMnO_6

104. D. Puggioni, A. Filippetti, and **V. Fiorentini**:
Antiferromagnetism and cuprate-like Fermi surface in a digital superlattice

105. G. M. Lopez, M. B. Maccioni, M. Scarrozza, A. Filippetti, and **V. Fiorentini**:
Multiferroicity and magnetoelectricity in $La_2Mn_2O_7$,

106. M. Scarrozza, G. M. Lopez, A. Filippetti, and **V. Fiorentini**:
Multiferroicity in vanadium-doped $La_2Ti_2O_7$

107. M. Scarrozza, A. Filippetti, and **V. Fiorentini**:
Diluted-magnetic doping of the $La_2Ti_2O_7$ structural ferroelectric

108. G. M. Lopez, E. Cadelano, and **V. Fiorentini**:
Ab initio structure, defects, and formation enthalpy of alumina-hafnia mixtures

C – Invited [7] and contributed [11] papers in peer-reviewed books

1. G. Pourtois, S. Clima, K. Sankaran, P. Delugas, **V. Fiorentini**, W.Magnus, B. Sorée, S. Van Elshocht, C. Adelman, J. Van Houdt, D. Wouters, S. De Gendt, M. M. Heyns, and J. Kittl:
Modeling of Alternative High-κ Dielectrics for Memory Based Applications,
invited paper (best symposium paper award) in S. Kar, M. Houssa, S. Van Elshocht, D. Landheer (ed.), *Physics and Technology of High-k Gate Dielectrics 7*, ECS Trans. **25**, p.131 (Electrochemical Society, Pennington 2009)

2. P. Delugas, **V. Fiorentini**, and A. Filippetti:
First-principles calculations on high-κ dielectric materials,
invited paper in L. Mitoseriu (ed.), *New Developments in Advanced Functional Ceramics* (Transworld Research Network, Kerala 2007)

3. P. Delugas, **V. Fiorentini**, and A. Filippetti:
Dielectric properties of rare-earth oxides : general trends from theory,
invited paper in M. Fanciulli and G. Scarel (eds.), *Rare Earth Oxide Thin Films: Growth, Characterization, and Applications*, Topics Appl. Physics **106**, 225-246 (Springer, Berlin 2006).

4. **V. Fiorentini**, P. Delugas, and A. Filippetti:
A theoretical view on the dielectric properties crystalline and amorphous high-κ materials and films,
invited paper in Ch.12, p.269-292, of *Advanced Gate Stacks for High-Mobility Semiconductors*,
edited by A. Dimoulas, E. Gusev, P. C. McIntyre, and M. Heyns, Series in Advanced Microelectronics vol.27 (Springer, Berlin, 2007).

5. A. Filippetti, **V. Fiorentini**, and G. M. Lopez:
Electronic Structure Of Defects In Dielectrics With Electronic Correlation,
invited paper in *Physics and Technology of High-k Dielectrics - IV*,
ECS Trans. **3** (Electrochemical Society, Pennington 2006)

6. P. Delugas, **V. Fiorentini**, A. Filippetti, and G. Pourtois:
Dielectric Properties Of High-κ Materials : A Theoretical View,
invited paper in *Physics and Technology of High-k Dielectrics - IV*,
ECS Trans. **3**, (Electrochemical Society, Pennington 2006)

7. M. Alessandri, R. Piagge, S. Alberici, E. Bellandi, M. Caniatti, G. Ghidini, A. Modelli, G. Pavia, E. Ravizza, A. Sebastiani, C. Wiemer, S. Spiga, M. Fanciulli, E. Cadelano, G. M. Lopez, and **V. Fiorentini**:
High-k materials in FLASH memories,
invited paper in *Physics and Technology of High-k Gate Dielectric III*,
ECS Trans. **1**, (Electrochemical Society, Pennington 2005).

8. P. Alippi, **V. Fiorentini**, and A. Filippetti:
Electronic Structure of bulk and defected $CaCu_3Ti_4O_{12}$, invited paper in *Physics and Technology of High-k Dielectrics - IV*,
ECS Trans. **3**, 291 (Electrochemical Society, Pennington 2006)

9. A. Bosin, **V. Fiorentini**, A. Lastri and G. B. Bachelet:
Pseudohamiltonians and Quantum Montecarlo,
in *Materials Theory and Modelling*,
edited by P. D. Bristowe, J. Broughton and J. M. Newsam,
MRS Proceedings **291**, 21-26 (1993).

10. S. Oppo, **V. Fiorentini** and M. Scheffler:
Surface alloying and surfactant action of Sb on Ag (111),
in *Mechanisms of Thin Film Formation*,
edited by S. M. Yalisove, C. V. Thompson and D. J. Eaglesham,
MRS Proceedings **317**, 323-328 (1994).

11. M. Scheffler, **V. Fiorentini**, and S. Oppo:
Growth of Metals and the Role of Surfactants,
in *Surface Science - Principles and Current Applications*
edited by R. J. MacDonald, E. C. Taglauer, K. R. Wandelt (Springer, Berlin 1996), p.219-231.

12. G. Cappellini, **V. Fiorentini**, K. Tenelsen, and F. Bechstedt:
Structure and quasiparticle energies of cubic, wurtzite and hexagonal BN,
in *Gallium Nitride and related compounds*,
edited by R. D. Dupuis, J. A. Edmond, F. Ponce and S. Nakamura,
MRS Proceedings **395**, 429-434 (1996).

13. A. Bosin, **V. Fiorentini**, and D. Vanderbilt:
Hydrogen, acceptors, and hydrogen-acceptor complexes in GaN,
in *Gallium Nitride and related compounds*,
edited by R. D. Dupuis, J. A. Edmond, F. Ponce and S. Nakamura,
MRS Proceedings **395**, 503-508 (1996).

14. A. Satta, **V. Fiorentini**, A. Bosin, F. Meloni and D. Vanderbilt:
Structural and electronic properties of AlN, GaN and InN, and band offsets at AlN/GaN ($10\bar{1}0$) and (0001) interfaces,
in *Gallium Nitride and related compounds*,
edited by R. D. Dupuis, J. A. Edmond, F. Ponce and
S. Nakamura, MRS Proceedings **395**, 515-520 (1996).

15. S. Serra, L. Miglio, and **V. Fiorentini**:
Simulated thermal properties of solid and amorphous gallium nitride,
in *Gallium Nitride and related compounds*,
edited by R. D. Dupuis, J. A. Edmond, F. Ponce and S. Nakamura,
MRS Proceedings **395**, 435-440 (1996).

16. A. Filippetti, **V. Fiorentini**, K. Stokbro, R. Valente, and S. Baroni:
Formation energy, relaxations, and stress of low index Rh surfaces,
in *Materials Theory, Simulations, and Parallel Algorithms*,
edited by E. Kaxiras and J. D. Johannopoulos,
MRS Proceedings **408**, 457-462 (1996).

17. **V. Fiorentini**, M. Methfessel, and S. Oppo:
Ab initio core-level shifts in metallic alloys,
in *Materials Theory, Simulations, and Parallel Algorithms*,
edited by E. Kaxiras and J. D. Johannopoulos,
MRS Proceedings **408**, 495-501 (1996).

18. F. Bernardini, **V. Fiorentini**, and D. Vanderbilt:
Offsets and polarization at strained AlN/GaN polar interfaces,
in *III-V Nitrides*,
edited by F.A. Ponce, T.D. Moustakas, I. Akasaki, and B.A. Monemar,
MRS Proceedings **449**, 923-928 (1997).

D – Papers [8] without peer review

1. **V. Fiorentini**, A. Satta, D. Vanderbilt, S. Massidda, and F.Meloni:
Semicore effects in gallium nitride,
in *The Physics of Semiconductors*,
edited by D. J. Lockwood, (World Scientific, Singapore, 1995), p.137-140.

2. **V. Fiorentini**, M. Methfessel and M. Scheffler:
Surface stress, relaxation, and reconstruction in fcc transition metals,
Il Vuoto **24**, 21-24 (1995)

3. S. Oppo, **V. Fiorentini** and M. Scheffler:
Size-effect surfactants for metal-on-metal growth: Sb on Ag (111),
Il Vuoto **24**, 37-39 (1995)

4. D. Fois, **V. Fiorentini** and S. Oppo:
Ga on Al (100) and hit-and-stick Al diffusion: a new surfactant for metals ?,
Il Vuoto **25**, 78-81 (1996).

5. **V. Fiorentini**, F. Bernardini, A. Bosin, and D. Vanderbilt:
Ab initio shallow acceptor levels in gallium nitride,
in *The Physics of Semiconductors*,
edited by M. Scheffler and R. Zimmermann (World Scientific, Singapore, 1996), p.2877-2880.

6. F. Bernardini, **V. Fiorentini**, and R. Nieminen:
Zn-related deep centers in wurtzite GaN,
in *The Physics of Semiconductors*,
edited by M. Scheffler and R. Zimmermann (World Scientific, Singapore, 1996), p.2881-2884.

7. **V. Fiorentini**, A. Bosin, S. Oppo, A. Satta, A. Filippetti, and D. Fois:
Ab-initio studies of material properties of wide-gap semiconductors, metal surfaces, and intermetallic alloys on vector and parallel supercomputers,
in *Science and Supercomputing*,
edited by G. Erbacci and M. Voli (CINECA, Bologna 1996), p.527-534.

8. F. Meloni, F. Bernardini, and **V. Fiorentini**:
Spontaneous polarization fields in III-V nitride nanostructures,
in *Blue Lasers and Light Emitting Diodes – II*,
edited by K. Onabe, K. Hiramatsu, K. Itaya, and Y. Nakano (Ohmsha, Tokio 1998), p.658-659.

E – Dissertations [2]

1. **V. Fiorentini**, *Studio teorico di accettori doppi in Ge*, Tesi di Laurea, Università degli Studi di Trieste, 1987 [in Italian, available upon request. Partially published in paper n.1 of Section B].

2. **V. Fiorentini**, *Eccitazioni elettroniche in semiconduttori*, Tesi di Dottorato di Ricerca, 1991 [in Italian, available upon request. Partially published in papers n.2, 3, 4, 5, 11, 12 of Section B, and n.9 of Section C.].

F – Other (errata, reply to comments, ...) [3]

1. **V. Fiorentini**, M. Methfessel and M. Scheffler:
Erratum: Reconstruction mechanism of fcc transition-metal (001) surfaces,
Phys. Rev. Lett. **81**, 2114-2114 (1998).

2. **V. Fiorentini** and M. Methfessel:
Reply to "Comment on Extracting convergent surface energies from slab calculations*"*,
J. Phys. Cond. Matter **10**, 895-895 (1998).

3. F. Bernardini and **V. Fiorentini**:
Erratum: Nonlinear macroscopic polarization in III-V nitride alloys,
Phys. Rev. B **65**, 129903 (2002).