

# Fabio Bernardini

## PUBLICATION LIST

---

### Book chapters

---

1) **Fabio Bernardini:**

*Spontaneous and Piezoelectric Polarization: Basic Theory vs. Practical Recipes*, in  
"Nitride Semiconductor Devices: Principles and Simulation",  
J. Piprek, Editor, Wiley-VCH, Weinheim, Germany (2007).

---

### Regular Papers (no proceedings)

---

- 1) C.M. Bertoni, M. Buongiorno Nardelli, **F. Bernardini**, F. Finocchi and E. Molinari:  
*Chemisorption of H on GaAs(110) : a first-principle calculation*,  
Europhysics Letters **13**, 653-8 (1990).
- 2) C.M. Bertoni, F. Finocchi, **F. Bernardini**, M. Buongiorno Nardelli:  
*Hydrogen on semiconductor surfaces: theory of the electronic structure*,  
Physica B, **170**, 429-35 (1991).
- 3) M. Buongiorno Nardelli, F. Finocchi, M. Palummo, R. De Felice, C.M. Bertoni, **F. Bernardini** and S. Ossicini:  
*Hydrogen covered Si(111) surfaces*,  
Surface Science **269/270**, 879-85 (1992).
- 4) S. Ossicini, and **F. Bernardini**:  
*Fermi-level pinning and interface states at Pb-Si(111) interface*,  
Solid State Communications **82**, 863-6 (1992).
- 5) A. Fasolino, S. Ossicini, **F. Bernardini**:  
*Electronic structure of thin Si layers in CaF<sub>2</sub>: hybridization versus confinement*,  
Solid State Electronics **37**, 1145-7 (1994).
- 6) **F. Bernardini**, A. Fasolino, S. Ossicini:  
*First-principle investigation of the electronic structure of Si-based layered structures*,  
Surface Science **307-309**, 984-8 (1994).

- 7) S. Ossicini, A. Fasolino, and **F. Bernardini**:  
*Si/CaF<sub>2</sub> Superlattices: A Direct Gap Structure Due to Interface State Coupling*,  
*Phys. Stat. Sol. (b)* **190**, 117-22 (1995).
- 8) S. Ossicini, A. Fasolino, **F. Bernardini**:  
*Gap opening in ultra-thin Si layers: role of confined and interface states*, *Phys. Rev. Lett.* **72**, 1044-7 (1994).
- 9) F. Arnaud d'Avitaya, L. Vervoort, F. Bassani, Stefano Ossicini, A. Fasolino, **F. Bernardini**:  
*Light emission at room temperature from Si/CaF<sub>2</sub> multilayers*,  
*Europhysics Letters* **31**, 25-30 (1995).
- 10) L. Dorigoni, O. Bisi, **F. Bernardini** and S. Ossicini:  
*Electron states and luminescence transition in porous silicon*,  
*Phys. Rev. B* **53**, 4557-64 (1996).
- 11) **F. Bernardini** and R. M. Nieminen:  
*Valence-band offset at the Al<sub>x</sub>Ga<sub>0.5-x</sub>In<sub>0.5</sub>P-ZnSe(001) lattice-matched interface*,  
*Phys. Rev. B* **55**, 1718-23 (1997).
- 12) A. Lindell, M. Pessa, A. Salokatve, **F. Bernardini**, R.M. Nieminen, M. Paalanen:  
*Band offset at the GaInP/GaAs heterojunction*,  
*Journal of Appl. Phys.* **82**, 3374-80 (1997).
- 13) **F. Bernardini**, V. Fiorentini and A. Bosin:  
*Theoretical evidence for efficient p-type doping of GaN using beryllium*, *Appl. Phys. Lett.* **70**, 2990-2 (1997).
- 14) **F. Bernardini**, V. Fiorentini and D. Vanderbilt:  
*Spontaneous polarization and piezoelectric constants of III-V nitrides*, *Phys. Rev. B* **56** , R10024-7 (1997).
- 15) **F. Bernardini**, V. Fiorentini and D. Vanderbilt:  
*Polarization-based calculation of the dielectric tensor of polar crystals*, *Phys. Rev. Lett.* **79** , 3958-61 (1997).
- 16) **F. Bernardini**, V. Fiorentini:  
*Macroscopic polarization and band offsets at nitride heterojunctions* *Phys. Rev. B* **57**, R9427-30 (1998).
- 17) **F. Bernardini** and V. Fiorentini:  
*Electronic dielectric constants of insulators calculated by the polarization method*,  
*Phys. Rev. B* **58**, 15292-5 (1998).
- 18) Antonella Fara, **F. Bernardini**, and V. Fiorentini:  
*Theoretical evidence for the semi-insulating character of AlN*,  
*J. of Appl. Phys.* **85**, 2001-3 (1999).

- 19) Fabio Della Sala, Aldo Di Carlo, Paolo Lugli, **Fabio Bernardini**, Vincenzo Fiorentini, Reinhard Scholz and Jean-Marc Jancu:  
*Free-carrier screening of polarization fields in wurtzite GaN/InGaN laser structures*, Appl. Phys. Lett. **74**, 2002-4 (1999).
- 20) Vincenzo Fiorentini, **Fabio Bernardini**, Fabio Della Sala, Aldo Di Carlo, and Paolo Lugli:  
*Effects of macroscopic-polarization in III-V nitrides multiple quantum wells*, Phys. Rev. B **60**, 8849 (1999).
- 21) **Fabio Bernardini**, Vincenzo Fiorentini:  
*Spontaneous versus Piezoelectric Polarization in III-V Nitrides: Conceptual Aspects and Practical Consequences.* , Phys. Stat. Sol. (b) **216**, 391-8 (1999).
- 22) **Fabio Bernardini**, Vincenzo Fiorentini:  
*Polarization fields in nitride nanostructures: ten points to think about*, Appl. Surf. Sci. **166**, 23-9 (2000).
- 23) **Fabio Bernardini**, Vincenzo Fiorentini:  
*Incorporation, diffusion, and electrical activity of Li in GaN*, Phys. Rev. B **61**, 12598-601 (2000).
- 24) Aldo Di Carlo, Fabio Della Sala and Paolo Lugli, Vincenzo Fiorentini, **Fabio Bernardini**:  
*Doping screening of polarization fields in nitride heterostructures*, Appl. Phys. Lett. **76**, 3950-2 (2000).
- 25) **Fabio Bernardini**, Maria Peressi, Vincenzo Fiorentini:  
*Band offsets and stability of BeTe/ZnSe (100) heterojunctions*, Phys. Rev. B **62**, R16302-5 (2000).
- 26) Carlo M. Carbonaro, Vincenzo Fiorentini, **Fabio Bernardini**:  
*Proof of the thermodynamical stability of the E' center in SiO<sub>2</sub>*, Phys. Rev. Lett. **86**, 3064-7 (2001).
- 27) **Fabio Bernardini**, Vincenzo Fiorentini, and David Vanderbilt:  
*Accurate calculation of polarization-related quantities in semiconductors*, Phys. Rev. B **63**, 193201-5 (2001).
- 28) Agostino Zoroddu, **Fabio Bernardini**, Paolo Ruggerone, and Vincenzo 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 (2001).

- 29) **Fabio Bernardini**, Vincenzo Fiorentini:  
*Nonlinear macroscopic polarization in III-V nitride alloys*,  
Phys. Rev. B **64**, 085207 (2001).
- 30) G. Satta, G. Profeta, **F. Bernardini**, A. Continenza, and S. Massidda:  
*Electronic and structural properties of superconducting MgB<sub>2</sub>, CaSi<sub>2</sub>, and related compounds*,  
Phys. Rev. B **64**, 104507 (2001).
- 31) G. Profeta, A. Continenza, **F. Bernardini**, and S. Massidda:  
*MgB<sub>2</sub> and BeB<sub>2</sub>: A comparative study of their electronic and superconducting properties*,  
Phys. Rev. B **65**, 054502 (2002).
- 32) Vincenzo Fiorentini, **Fabio Bernardini**, and Oliver Ambacher:  
*Evidence for nonlinear macroscopic polarization in III-V nitride alloy heterostructures*,  
Appl. Phys. Lett. **80**, 1204 (2002).
- 33) O. Ambacher, J. Majewski, C. Miskys, A. Link, M. Hermann, M. Eickhoff, M. Stutzmann, **F. Bernardini**, V. Fiorentini, V. Tilak, B. Schaff and L. F. Eastman:  
*Pyroelectric properties of Al(In)GaN/GaN hetero- and quantum well structures*,  
J. Phys.: Condens Matter **14**, 3399-3434 (2002).
- 34) C.M. Carbonaro, V. Fiorentini, and **F. Bernardini**:  
*Stability of Ge-related point defects and complexes in Ge-doped SiO<sub>2</sub>*,  
Phys. Rev. B **66**, 233201 (2002).
- 35) **F. Bernardini**, V. Fiorentini:  
*First-principles calculation of the piezoelectric tensor d of III–V nitrides*,  
Appl. Phys. Lett. **80**, 4145 (2002).
- 36) A. Mattoni, **F. Bernardini**, and L. Colombo:  
*Self-interstitial trapping by carbon complexes in crystalline silicon*,  
Phys. Rev. B. **66**, 195214 (2002).
- 37) G. Profeta, A. Continenza, **F. Bernardini**, and S. Massidda:  
*Electronic and dynamical properties of the MgB<sub>2</sub> surface: Implications for the superconducting properties*,  
Phys. Rev. B. **66**, 184517 (2002).
- 38) G. Profeta, A. Continenza, **F. Bernardini**, G. Satta and S. Massidda:  
*Electronic and dynamical properties of MgB<sub>2</sub> and related compounds*,  
International Journal of Modern Physics B. **16**, 1563 (2002).

- 39) **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).
- 40) O. Ambacher, M. Eickhoff, A. Link, M. Hermann, M. Stutzmann, **F. Bernardini**, V. Fiorentini, Y. Smorchkova, J. Speck, U. Mishra, W. Schaff, V. Tilak, and L.F. Eastman:  
*Electronics and sensors based on pyroelectric AlGaN/GaN heterostructures,*  
Phys. Stat. Sol. (c) **6**, 1878-1907 (2003).
- 41) **F. Bernardini**, G. Profeta, and A. Continenza:  
*Bi incorporation in GaN and  $Al_xGa_{1-x}N$  alloys,*  
Phys. Rev. B **68**, 195205 (2003).
- 42) **F. Bernardini**, S. Picozzi, and A. Continenza: *Energetic stability and magnetic properties of Mn dimers in silicon*, Appl. Phys. Lett. **84**, 2289 (2004).
- 43) **F. Bernardini**, A. Mattoni, and L. Colombo:  
*Energetics of native point defects in cubic silicon carbide,*  
Eur. Phys. J. B. **38**, 437-444 (2004).
- 44) **F. Bernardini** and L. Colombo:  
*Interaction of doping impurities with the 30 partial dislocations in SiC: An ab initio investigation,*  
Phys. Rev. B **72**, 085215 (2005).
- 45) **F. Bernardini** and S. Massidda:  
*Anomalous effect of Li-Al codoping in MgB<sub>2</sub>: A simple explanation,*  
Phys. Rev. B **74**, 014513 (2006).
- 46) R. S. Gonnelli, D. Daghero, G. A. Ummarino, A. Calzolari, M. Tortello, V. A. Stepanov, N. D. Zhigadlo, K. Rogacki, J. Karpinski, **F. Bernardini**, and S. Massidda:  
*Effect of Magnetic Impurities in a Two-Band Superconductor: A Point-Contact Study of Mn-Substituted MgB<sub>2</sub> Single Crystals,*  
Phys. Rev. Lett. **97**, 037001 (2006).
- 47) **F. Bernardini** and S. Massidda:  
*First-principle investigation of native and impurity defects in MgB<sub>2</sub>,*  
Europhysics Letters **76** (3), 491-7 (2006).

---

## Conference Proceedings

---

- 1) C.M. Bertoni, M. Buongiorno Nardelli, **F. Bernardini**, F. Finocchi and E. Molinari:  
*Structure and Vibrational Properties of Hydrogen on GaAs(110): First Principles Results*,  
*Proceedings of the 21th International Conference on the Physics of Semiconductors*.  
ed. by E.M. Anastassakis and J.D. Joannopoulos,  
(World Scientific, Singapore, 1990), pp. 163-6.
- 2) S. Ossicini, A. Fasolino, **F. Bernardini**:  
*Electronic properties of low dimensional silicon structures*,  
in "Optical Properties of Low Dimensional Silicon Structures" ed. D. Bensahel, L. P. Canham and S. Ossicini, Kluwer Academic Publishers, Dordrecht, The Netherlands,(1993), pp. 219-28.
- 3) **F. Bernardini** and R. M. Nieminen:  
*Valence-band offset at the Zn-P interface between ZnSe and III-V wide gap semiconductor alloys: a first-principles investigation*,  
in "Materials Theory, Simulations, and Parallel Algorithms", Material Research Society Proc. Vol. **408**, edited by E. Kaxiras, J. Joannopoulos, P. Vashista, R.V. Kalia, (Material Research Society, Pittsburg, Pennsylvania,USA), pp. 539-44 (1996).
- 4) V. Fiorentini, **F. Bernardini**, A. Bosin, and D. Vanderbilt:  
*Ab initio shallow acceptor levels in gallium nitride*,  
in *The Physics of Semiconductors*, edit by M. Scheffler and R. Zimmerman (World Scientific, Singapore, 1996, ISBN: 981-02-2936-4), p. 2877-80.
- 5) **F. Bernardini**, V. Fiorentini, and R. Nieminen:  
*Zn-related deep centers in wurtzite GaN*,  
in *The Physics of Semiconductors*, edit by M. Scheffler and R. Zimmerman (World Scientific, Singapore, 1996, ISBN: 981-02-2936-4), p. 2881-4.
- 6) **F. Bernardini**, V. Fiorentini, and D. Vanderbilt:  
*Offsets and polarization at strained AlN/GaN polar interfaces*,  
in "III-V Nitrides", (MRS Proceedings Vol. **449**), F.A. Ponce, T.D. Moustakas, I. Asaki, and B.A. Monemar, eds. (Material Research Society, Pittsburgh, PA, 1997), pp. 923-28 (1997).
- 7) G. Profeta, A. Continenza, **F. Bernardini**, M. Monni, and S. Massidda:  
*Electronic, dynamical and superconducting properties of MgB<sub>2</sub>: doping, surface and pressure effects*,  
Superconductor Science and Technology **16**, 137-142 (2003).

- 8) G. Profeta, A. Continenza, **F. Bernardini**, G. Satta, and S. Massidda: *Electronic and structural properties of superconducting MgB<sub>2</sub> and related systems*, in *Superconducting Magnesium Diboride: Studies of High Temperature Superconductors*, edit by A.V. Narlikar, (NOVA Publishers, Hauppauge, NY, USA, 2002, ISBN: 1-59033-131-1), pp. 117-134.
- 9) M. Salvador, J.M. Perlado, A. Mattoni, **F. Bernardini**, L. Colombo: *Defect energetics of  $\beta$ -SiC using a new tight-binding molecular dynamics model*, Journal of Nuclear Materials, **329-333**, 1219 (2004).
- 10) **F. Bernardini**, M. Monni, A. Sanna, Sandro Massidda: *Electronic and structural properties of LiAl co-doped MgB<sub>2</sub>*, Physica C, **460-462**, 566 (2007).

---

## Dissertations

---

- 1) **F. Bernardini**, *Calcolo da Principi Primi delle Proprietà Elettroniche, Strutturali e Vibrazionali per Solidi, Superfici e Chemisorbimento Ordinato*, Tesi di Laurea, Università di Roma "Tor Vergata", 1990.
- 2) **F. Bernardini**, *Studio da Principi Primi delle Proprietà Elettroniche di Interfacce e Sistemi Confinati basati sul Silicio*, Tesi di Dottorato di Ricerca, Università di Modena, 1994.
-