



## NANOPHASE Network Publications

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***NANOPHASE-related publications by NANOPHASE groups and their members, up to the end of the network on 31.5.04.***

(If any non-NANOPHASE-team, duplicate listings, or other errors have crept into this list, please inform Rex Godby)

- ***Added 1 June 1999***

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  - "Evaluation of GW approximations for the self-energy of a Hubbard cluster", C. Verdozzi, R.W. Godby and S. Holloway, *Phys. Rev. Lett.* **74** 2327 (1995).
  - "Density-polarisation functional theory of the response of a periodic insulating solid to an electric field", X. Gonze, P. Ghosez and R.W. Godby, *Phys. Rev. Lett.* **74** 4035 (1995).
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  - C.-O. Almbladh and M. Hindgren, *Vertex corrections beyond the *GW* approximation in polaron models*, to be published
  - U. von Barth, C.-O. Almbladh, and P. S. Svendsen, *Second-Order Perturbation Theory as Applied to Impurities in the Electron Gas*, to be published
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### **Joint NANOPHASE publications 1.6.00-5.3.03 added 5.3.03**

- **J101**. "GaAs(001): Surface structure and optical properties", W.G. Schmidt [Jena], F. Bechstedt [Jena] G. Onida [Milan] *phys. stat. sol. (a)* **188**, 1401 (2001) (9 pages).
- **J103**. "Theory of modeling the optical properties of surfaces", G. Onida [Milan], W.G. Schmidt [Jena], O. Pulci [Rome], M. Palummo [Rome], **A. Marini [Rome; now NANOPHASE-funded Young Researcher in San Sebastián], C. Hogan [Rome; NANOPHASE-funded Young Researcher]**, R. Del Sole [Rome], *phys. stat. sol. (a)* **188**, 1233 (2001) (10 pages).
- **M1**. "The GaAs(100) surface: A new perspective from Energy Loss Spectra", A. Balzarotti, M. Fanfoni, F. Patella, F. Arciprete, E. Placidi, G. Onida [Milan], R. Del Sole [Rome], *Surface Science* Vol. 524 L71 (2003).
- **M2** "Image resonance in the many-body density of states at a metal surface", G. Fratesi [Milan], G.P. Brivio [Milan], P. Rinke [York] and R.W. Godby [York], submitted (2003).
- **P1**. "Electronic Excitations: Density-Functional versus Many-body Green's Functions Approaches", G. Onida [Milan], L. Reining [Paris], and A. Rubio [San Sebastián], *Reviews of Modern Physics* **74** 601 (2002) (59 pages)
- **P12**. "*Ab initio* pseudopotential calculation of the equilibrium structure of tin monoxide" M. Meyer [Paris], G. Onida [Milan], M. Palummo [Rome], and L.

Reining [Paris], Phys. Rev. B **64**, 045119 (2001).

- **P15.** "Long-range contribution to the exchange-correlation kernel of time-dependent density functional theory", Silvana Botti [Paris], Francesco Sottile [Paris], Nathalie Vast [Paris], Valerio Olevano [Paris], Lucia Reining [Paris], Angel Rubio [San Sebastián, Paris], Giovanni Onida [Milan], Rodolfo Del Sole [Rome] and R.W. Godby [York], submitted. (16 pages)
- **P16.** "Optical and loss spectra of carbon nanotubes: depolarization effects and intertube interactions", A.G. Marinopoulos [Paris: NANOPHASE-funded Young Researcher], L. Reining [Paris], A. Rubio [San Sebastián, Paris], and N. Vast [Paris], submitted. (4 pages)
- **P2.** "Excitonic effects in solids described by time-dependent density functional theory", L. Reining [Paris], V. Olevano [Paris], A. Rubio [San Sebastián] and G. Onida [Milan], Phys. Rev. Lett. **88**, 066404 (2002); cond-mat/0109434. (4 pages)
- **P3.** "Anisotropy and interplane interactions in the dielectric response of graphite", **A.G. Marinopoulos [Paris: NANOPHASE-funded Young Researcher]**, L. Reining [Paris], V. Olevano [Paris], A. Rubio [San Sebastián], T. Pichler, X. Liu, M. Knupfer and J. Fink, Phys. Rev. Lett. **89**, 076402 (2002). (4 pages)
- **P4.** "Excitonic Effects on the Silicon Plasmon Resonance", V. Olevano [Rome, Paris] and L. Reining [Paris], Phys. Rev. Lett. **86**, 5962 (2001). (4 pages)
- **P5.** "Long range behavior and frequency dependence of exchange-correlation kernels for response functions in solids", R. Del Sole and G. Adragna [Rome], and V. Olevano and L. Reining [Paris], Phys. Rev. B **67**, 045207 (2003). (5 pages)
- **P6.** "Can optical spectroscopy directly elucidate the ground state of C<sub>20</sub>?", A. Castro, **M.A.L. Marques [San Sebastián: NANOPHASE-funded Young Researcher]**, J.A Alonso, G.F. Bertsch, K. Yabana and A. Rubio [San Sebastián, Paris], Journal of Chemical Physics **116**, 1930-1934 (2002)
- **P7.** "Many-body effects on one-electron energies and wavefunctions in low dimensional systems", O. Pulci [Rome], L. Reining [Paris], G. Onida [Milan], R. Del Sole [Rome], and F. Bechstedt [Jena], Comp. Mat. Science **20**, 300 (2001).
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- **R12.** "Structural and optical properties of the Ge(111)-(2x1) surface", M. Rohlfing, M. Palummo [Rome], G. Onida [Milan], R. Del Sole [Rome], Phys. Rev.

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- **R13.** "Plane-waves DFT-LDA calculation of the electronic structure and absorption spectrum of Copper", **A. Marini [Rome; now NANOPHASE-funded Young Researcher in San Sebastián]**, G. Onida [Milan] and R. Del Sole [Rome], Phys. Rev. B **64**, 195125 (2001)
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- **R17.** "Calculation of surface Second Harmonic Generation vs. experiment: Si(111)1x1 H as a test case", J.J. E. Meija, B. S. Mendoza, M. Palummo [Rome], G. Onida [Milan], R. Del Sole [Rome], S. Bergfeld, W. Daum, Phys. Rev. B **66**, 195329 (2002)
- **R20.** "Ab-initio calculation of the optical properties of BN(110)", G. Cappellini, G. Satta, M. Palummo [Rome], G. Onida [Milan], Phys. Rev. B **66**, 115 412 (2002)
- **R21.** "Optical properties of Ge quantum dots", M. Palummo [Rome], G. Onida [Milan], R. Del Sole [Rome], A. Stella, P. Tognini, P. Cheyssac [Rome], Phys. St. Sol. (b) **224**, 247 (2001)
- **R224.** "Finite Temperature "ab-initio" simulation of solids: Ground-state properties and electronic spectra from Car-Parrinello molecular Dynamics", by **C. Hogan [Rome: NANOPHASE-funded Young Researcher]**, G. Onida[Milan] , and R. Del Sole[Rome], in "Radiation-Matter Interaction in Confined Systems", ed. by L.C. Andreani, G. Benedek, E. Molinari, Pages 57-72, S.I.F., Bologna, Italy, 2002.
- **R225** "Optical properties of real surfaces from microscopic calculations of the dielectric function of finite atomic slabs" C. Hogan [Rome: NANOPHASE-funded Young Researcher], R. Del Sole [Rome], G. Onida [Milan], Phys. Rev. B submitted (2003)
- **R226** "Dynamical excitons in metals and semiconductors" **A. Marini [Rome: now NANOPHASE-funded Young Researcher in San Sebastián]**, R. Del Sole [Rome] submitted (2003)
- **R227** "All-electron versus pseudopotential calculation of optical properties: The case of GaAs", P. Monachesi [Rome], **A. Marini [Rome: now NANOPHASE-funded Young Researcher in San Sebastián]**, G. Onida[Milan], M. Palummo [Rome], and R. Del Sole [Rome], phys. stat. sol. A **184** 101 (2001).



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- **R6**. “Quasiparticle bandstructure effects on the lifetimes of *d* holes in copper within the *GW* approximation”, **A. Marini [Rome; now NANOPHASE-funded Young Researcher in San Sebastián]**, R. Del Sole [Rome], A. Rubio [San Sebastián] and G. Onida [Milan], Phys. Rev. B **66**, 161104R (2002)
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- **B102** “Quantum Monte Carlo calculations of H<sub>2</sub> dissociation on Si(001)”, C. Filippi, S. B. Healy, P. Kratzer, E. Pehlke, and M. Scheffler [Berlin], Phys. Rev. Lett. **89**, 166102 (2002).
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- **B104** “Quasiparticle calculations for point defects on semiconductor surfaces”, M. Hedström, A. Schindlmayr, and M. Scheffler, phys. stat. sol. (b) **234**, 346 (2002).
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- **Y54**. "Self-consistent calculation of total energies of the electron gas using many-body perturbation theory", P. García-González [York] and R.W. Godby [York], Phys. Rev. B **63** 075112 (2001) (*4 pages*). <<http://publish.aps.org/abstract/PRB/v63/e075112>>
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- **Y56**. "GW self-energy calculations for surfaces and interfaces" (review in special CCP3 issue), P. García-González [York] and R.W. Godby [York], Computer Physics Communications **137** 108-122 (2001).

### ***Joint NANOPHASE publications Year 3 (1.6.02-31.5.03) added 19.10.04***

- **P301 (N\*)** ``Anisotropy and interplane interactions in the dielectric response of graphite interactions in the dielectric response of graphite'', **A.G. Marinopoulos [Paris: NANOPHASE-funded Young Researcher]**, L. Reining [Paris], V. Olevano [Paris], A. Rubio [San Sebastián], T.Pichler, X. Liu, M. Knupfer, and J. Fink, Phys. Rev. Lett. **89**, 076402 (2002) (Task B4).
- **P304 (N\*)** ``Optical and loss spectra of carbon nanotubes: Depolarization effects and intertube interactions'', **A.G. Marinopoulos [Paris: NANOPHASE-funded young researcher]**, Lucia Reining [Paris], Angel Rubio [San Sebastián], Nathalie Vast [Paris], accepted, Phys. Rev. Lett. (Task B4).
- **R302 (N\*)** ``Long-range behavior and frequency dependence of exchange-correlation kernels in solids'', R. Del Sole [Rome], G. Adragna [Rome], V. Olevano [Paris], L. Reining [Paris], Phys. Rev. B **67**, 045207 (2003) .
- **R006 (N\*)** ``Quasiparticle bandstructure effects on the lifetimes of *d* holes in copper within the *GW* approximation'', A. Marini [Rome], R. Del Sole [Rome], A. Rubio [San Sebastián] and G. Onida [Rome], Phys. Rev. B **66**, 161104R (2002) .
- **S217 (N\*)** ``Optical absorption in small BN and C nanotubes'', L. Wirtz [San Sebastián], V. Olevano [Paris] A.G. Marinopoulos [Paris], L. Reining [Paris] and A. Rubio [San Sebastián], Electronic Properties of Novel Materials: XVIIth International Winterschool, Ed. H. Kuzmany, J. Fink, M. Mehring and S. Roth, World Scientific, Singapore (2003) (Task B4).

- **Y250 (N\*)** ``Density functional theories and self-energy approaches'', R.W. Godby [York] and P. García-González [San Sebastián], chapter in ``A Primer in Density Functional Theory'', ed. Carlos Fiolhais, Fernando Nogueira and M. A. L. Marques, Springer (Heidelberg), 2003 (Task A2).
- **L17 (N\*)** ``The Pd(100)  $\sqrt{5} \times \sqrt{5}$  R30° O surface oxide revised'', M. Todorova and E. Lundgren and V. Blum and **A. Mikkelsen [NANOPHASE Postdoc Lund]** and S. Gray and J. Gustafson and M. Borg and J. Rogal and K. Reuter and J. N. Andersen and M. Scheffler [Berlin], Surface Science (accepted) (Task C).
- **R314 (N\*)** ``Early stages of cesium adsorption on the As-rich  $c(2 \times 8)$  reconstruction of GaAs(001): Adsorption sites and Cs-induced chemical bonds'', **C. Hogan [Rome: NANOPHASE-funded Young Researcher]**, D. Paget, Y. Garreau, M. Sauvage, G. Onida [Rome] L. Reining [Paris], P. Chiaradia, V. Corradini, submitted (Task C4).
- **P250 (N\*)** ``Long-range contribution to the exchange-correlation kernel of time-dependent density functional theory'', Silvana Botti [Paris], Francesco Sottile [Paris], Nathalie Vast [Paris], Valerio Olevano [Paris], H. Weissker [Jena], Lucia Reining [Paris], Angel Rubio [San Sebastián], Giovanni Onida [Rome], Rodolfo Del Sole [Rome] and R.W. Godby [York], submitted (Tasks A5, B4, C4).
- **J301 (N\*)** ``P-rich GaP(001)(2 × 1)/(2 × 2) Surface - A Hydrogen-Adsorbate Structure'', P.H. Hahn [Jena], W.G. Schmidt [Jena], F. Bechstedt [Jena], O. Pulci [Rome], R. Del Sole [Rome], Phys. Rev. B (accepted) (Task C4).
- **S221 (N\*)** ``Dynamical excitonic effects in metals and semiconductors'', **A. Marini [San Sebastián: NANOPHASE-funded Young Researcher]**, R. Del Sole [Rome], submitted (Task A3).
- **R299 (N\*)** ``Ab-initio calculation of the exchange-correlation kernel in solids'', G. Adragna, R. Del Sole [Rome], **A. Marini [San Sebastián: NANOPHASE-funded Young Researcher]**, submitted .
- **J300 (N\*)** ``Many-body and overlayer effects on surface optical properties'', F. Bechstedt [Jena], R. Del Sole [Rome], S. Glutsch [Jena], P.H. Hahn [Jena], O. Pulci [Rome], W.G. Schmidt [Jena], phys. stat. sol. (b), accepted (14 pages) (Task C4).
- **Y251 (N\*)** ``Non-local image effects in quasiparticle wavefunctions and energies for jellium spheres'', P. Rinke [York], P. García-González [San Sebastián] and R.W. Godby [York], in preparation (Task A3).
- **P306 (N\*)** ``Ab initio Study of the Optical Absorption and wavevector-dependent Dielectric Response of Graphite'', **A.G. Marinopoulos [Paris: NANOPHASE-funded young researcher]**, L. Reining [Paris], A. Rubio [San Sebastián], V. Olevano [Paris], in preparation (Task B4).
- **Y252 (N\*)** ``GW total energy calculations for jellium spheres'', K.T. Delaney [York], P. Rinke [York], P. García-González [San Sebastián] and R.W. Godby [York], in preparation (Task A6).
- **B250 (N\*)** ``Image resonance in the many-body density of states at a metal surface, G. Fratesi, G.P. Brivio, P. Rinke [Berlin] and R.W. Godby [York] (Task submitted C2).
- **R304 (N\*)** ``Optical anisotropy induced by cesium adsorption on the As-rich



- $c(2 \times 8)$  reconstruction of GaAs(001)", **C. Hogan [Rome: NANOPHASE-funded Young Researcher]**, D. Paget, O.E. Tereschenko, L. Reining [Paris], and G. Onida [Rome], In preparation (Task C4).
- **R309 (N\*)** ``Strongly bound exciton at the C(100) surface'', M. Palumbo [Rome], O. Pulci [Rome], **A. Marini [San Sebastián, Young Researcher]**, R. Del Sole [Rome], V. Olevano [Paris], L. Reining [Paris], in preparation (Task C4).
  - **S220 (N\*)** ``Bound excitons in TDDFT'', **A. Marini [San Sebastián: NANOPHASE-funded Young Researcher]**, A. Rubio [San Sebastián] and R. Del Sole [Rome], in preparation (Task B4).

### **Other NANOPHASE publications Year 3 (1.6.02-31.5.03) added 19.10.04**

- **P303 (N)** ``Parameter-free calculation of response functions in time-dependent density functional theory'', F. Sottile [Paris], V. Olevano [Paris], L. Reining [Paris], accepted, Phys. Rev. Lett. (Task A5, B4, C4).
- **P305 (N)** ``Macroscopic and microscopic components of exchange-correlation interactions'', F. Sottile [Paris], K. Karlsson, L. Reining [Paris], F. Aryasetiawan, submitted, Phys. Rev. B (Task A5, B4, C4).
- **J203 (N)** ``Efficient  $O(N^2)$  method to solve the Bethe-Salpeter equation'', W.G. Schmidt [Jena], S. Glutsch [Jena], P. Hahn [Jena], F. Bechstedt [Jena], Phys. Rev. B **67**, 085307 (2003).
- **J303 (N)** ``Properties of interfaces between cubic and hexagonal polytypes of silicon carbide'', **C. Raffy [Jena: NANOPHASE-funded Young Researcher]**, J. Furthmüller [Jena], F. Bechstedt [Jena], J. Phys.: Condens. Matter **14**, 12725 (2002) (Task C4, A5).
- **J307 (N)** ``Quasiparticle band structures and optical properties of  $\beta$ -cristobalite  $\text{SiO}_2$ '', **L.E. Ramos [Jena: NANOPHASE-funded Young Researcher]**, J. Furthmüller [Jena], F. Bechstedt [Jena], Phys. Rev. B (submitted) (Task A5).
- **L328 (N)** ``Variational energy functionals tested on atoms'', N.E. Dahlen [Lund] and U. von Barth [Lund], submitted to Phys. Rev. B. (Task A).
- **L329 (N)** ``Variational MP2 theory'', N.E. Dahlen [Lund] and U. von Barth [Lund], submitted to Phys. Rev. B. (Task A).
- **S215 (N)** ``Structural and Thermal Properties of Silicon-doped Fullerenes'', P.A. Marcos, J.A. Alonso, A. Rubio [San Sebastián] and M.J. López, Journal of Chemical Physics **119**, 1127-1135 (2003) (Task A1).
- **S219 (N)** ``Direct Observation of the Mechanical Properties of Singlewall Carbon Nanotubes and their Junctions at the Atomic Level'', H.E. Troiani, M. Miki-Yoshida, G.A. Camacho-Bragado, M.A.L. Marques [San Sebastián], A. Rubio [San Sebastián], J.A. Ascencio and M. Jose-Yacaman, Nanoletters (Communication) **3(6)**, 751-755 (2003) (Task B1 and A1).
- **J306 (N)** ``Structural relaxation in Si and Ge nanocrystallites: Influence on the electronic and optical properties'', H.-Ch. Weissker [Jena], J. Furthmüller [Jena], F. Bechstedt [Jena], Phys. Rev. B **67**, 245304 (2003) (Task A5).
- **S213 (N)** ``Time-Dependent Density-functional approach for biological photoreceptors: the case of the Green Fluorescent Protein'', **M.A.L. Marques**

- [Nanophase founded Young researcher]**, X. Lopez, D. Varsano, A. Castro, and A. Rubio [San Sebastián], Physical Review Letters **90**, 158101-1,4 (2003) (Task A5 and B4).
- **Y201 (N)** ``Maximum-entropy theory of steady-state quantum transport'', **P. Bokes [York: NANOPHASE-funded Young Researcher]** and R. W. Godby [York], submitted; <<http://arxiv.org/abs/cond-mat/0301485>> (Task B3).
  - **Y253 (N)** ``Maximum-entropy theory of quantum transport - single-particle self-consistent field formalism'', **P. Bokes [York: NANOPHASE-funded Young Researcher]**, **H. Mera [York: NANOPHASE-funded Young Researcher]** and R. W. Godby [York], in preparation (Task B3).
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  - **R017 (N)** ``Surface second-harmonic generation from Si(111)(1 x 1)H: Theory versus experiment'', J. E. Mejía, B. S. Mendoza, M. Palummo [Rome], G. Onida [Rome], R. Del Sole [Rome], S. Bergfeld, and W. Daum, Phys. Rev. B **66**, 195329 (2002) (Task C4).
  - **R308 (N)** ``Origin of the broadening of surface optical transitions of As-rich and Ga-rich GaAs(001)'', D. Paget, O. E. Tereshchenko, A. B. Gordeeva, V. L. Berkovits, G. Onida [Rome], Surface Science **529**, p.204-214, 1-2 (2003) (Task C4).
  - **R310 (N)** ``The GaAs(001)- $c(4 \times 4)$  surface: a new perspective from energy loss spectra'', A. Balzarotti, M. Fanfoni, F. Patella, F. Arciprete, E. Placidi, G. Onida [Rome] and R. Del Sole [Rome], Surface Science Letters **524**, L71-L76 (2003) (Task C4).
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  - **R224 (N)** ``Finite Temperature "ab-initio" simulation of solids: Ground-state properties and electronic spectra from Car-Parrinello molecular Dynamics'', **C. Hogan [Rome: NANOPHASE-funded Young Researcher]**, G. Onida [Rome], and R. Del Sole [Rome], in: *Radiation-Matter Interaction in Confined Systems*, ed. by L.C. Andreani, G. Benedek, E. Molinari, Pages 57-72, S.I.F., Bologna, Italy, (2002). (Task C4).
  - **R225 (N)** ``Optical properties of real surfaces from microscopic calculations of the dielectric function of finite atomic slabs'', **C. Hogan [Rome: NANOPHASE-funded Young Researcher]**, R. Del Sole [Rome], G. Onida [Rome], Phys. Rev. B

- 68**, 035405-7, 3 (2003) (Task C3, C4).
- **J305 (N)** ``Adatoms, dimers and interstitial on group-IV (113) surfaces: First-principles studies of energetical, structural and electronic properties'', A.A. Stekolnikov [Jena], J. Furthmüller [Jena], F. Bechstedt [Jena], Phys. Rev. B **67**, 195332 (2003) (Task C4).
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  - **R230 (N)** ``GW calculations on surfaces: an application to the study of clean and Sb-covered Si(001)'', O. Pulci [Rome], J. Power, A. I. Shkrebtii, W. Richter, R. Del Sole [Rome], submitted Comp. Mat. Sci. (Task C4).
  - **R228 (N)** ``Surface and bulk origin of the optical anisotropy of As-rich GaAs(001) and Ga<sub>1-x</sub>In<sub>x</sub>As(001)'', D. Paget, **C. Hogan [Rome: NANOPHASE-funded Young Researcher]**, V. L. Berkovits, and O. E. Tereshchenko, Phys. Rev. B **67**, 245313 (2003) (Task C4).
  - **R301 (N)** ``Effect of adsorption of electronegative and electropositive elements on the surface optical anisotropy of GaAs(001)'', **C. Hogan [Rome: NANOPHASE-funded Young Researcher]**, D. Paget, O. E. Tereshchenko, R. Del Sole [Rome], accepted, phys. stat. sol. (a) (Task C4).
  - **R306 (N)** ``Surface versus bulk contributions from Reflectance Anisotropy and Electron Energy Loss Spectra of GaAs(001)-c(4 × 4) surface'', F. Arciprete, C. Goletti, E. Placidi, P. Chiaradia, M. Fanfoni, F. Patella, **C. Hogan [Rome: NANOPHASE-funded Young Researcher]** and A. Balzarotti, submitted to Phys. Rev. B (Task C4).
  - **R016 (N)** ``First-principles calculation of the plasmon resonance and of the reflectance spectrum of silver in the GW approximation'', Andrea Marini [Rome], Rodolfo Del Sole [Rome], and Giovanni Onida [Rome], Phys. Rev. B **66**, 115101 (2002) .
  - **R234 (N)** ``Ab initio calculation of depth resolved optical anisotropy of the Cu (110) surface'', P. Monachesi [Rome], M. Palumbo [Rome], R. Del Sole [Rome], A. Grechnev, O. Eriksson, Phys. Rev. B. (in press).
  - **R303 (N)** ``Cu(100) surface: high-resolution experimental and theoretical band mapping'', C. Baldacchini, L. Chiodo (Rome), F. Allegretti, C. Mariani, M. G. Betti, P. Monachesi (Rome), R. Del Sole (Rome), accepted Phys. Rev. B (Task C4).
  - **S218 (N)** ``Time and energy-resolved two photon-photoemission of the Cu(100) and Cu(111) metal surfaces'', D. Varsano, M.A.L. Marques [San Sebastián Nanophase Young Researcher] and A. Rubio [San Sebastián], Computational Material Science (in press 2003) (Task C2).
  - **R233 (N)** ``Ab initio calculation of Electron Energy Loss spectra of clean and 1ML Fe-covered Ni(111)'', R. Capelli, P Monachesi [Rome], R. Del Sole [Rome] and G.C. Gazzadi, Eur. Phys. J B 30, 117 (2002) (Task C4).
  - **L16 (N)** ``The identification of step atoms by high resolution core level spectroscopy'', J. Gustafson, M. Borg, V. Blum, **A. Mikkelsen [NANOPHASE Postdoc]**, S. Gorovikov, E. Lundgren and J. N. Andersen [Lund], Phys. Rev. Lett (accepted) (Task C).
  - **R231 (N)** ``Ab-initio investigation of the Adsorption of Organic Molecules at

- Si(111) and Si(100) surfaces", R. Di Felice, C.A. Pignedoli, C.M. Bertoni, A. Catellani, P.L. Silvestrelli, C. Sbraccia, F. Ancilotto, M. Palummo [Rome], O. Pulci [Rome], Surf. Sci. 532-535, 982 (2003) (Task C4).
- **R315 (N)** ``Ab-initio study of the adsorption of Acetylene on Si(001) surface", O. Pulci [Rome], P.L. Silvestrelli, M. Palummo [Rome], F. Ancelotto, R. Del Sole [Rome], submitted Phys. Stat. Solidi (Task C4).
  - **R316 (N)** ``Acetylene on Si(100) from first principles: the puzzle of the ``end bridge" structure", P.L. Silvestrelli, O. Pulci [Rome], M. Palummo [Rome], R. Del Sole [Rome], and F.Ancelotto, submitted PRB (Task C4).
  - **J308 (N)** ``Uracil adsorbed on Si(001): Structure and Energetics", K. Seino [Jena], W.G. Schmidt [Jena], M. Preuss [Jena], F. Bechstedt [Jena], J. Phys. Chem. B **107**, 5031 (2003) (Task C4).
  - **P302 (N)** ``Ab initio calculation of the dielectric tensor of GaAs/AlAs superlattices", S. Botti [Paris], N. Vast [Paris], L. Reining [Paris], V. Olevano [Paris], and L.C. Andreani, Phys. Rev. Lett. **89**, 216803 (2002) (Task C3,C4).
  - **P307 (N)** ``Origin of the anisotropy in the dielectric response of GaAs/AlAs superlattices", S. Botti [Paris], N. Vast [Paris], L. Reining [Paris], V. Olevano [Paris], L.C. Andreani, in preparation .
  - **J302 (N)** ``Principles of surface physics", F. Bechstedt [Jena], Springer-Verlag, Berlin 2003 (Task C4).
  - **R311 (N)** ``Theory of surface optical properties", R. Del Sole [Rome], M. Palummo [Rome], O. Pulci [Rome], to appear in 'Epioptics-7', World Scientific, ed. A. Cricienti. (Task C4).
  - **R313 (N)** ``First-principles optical spectra of semiconductor surfaces: from one-particle to many-body approach", M. Palummo [Rome], O. Pulci [Rome], R. Del Sole [Rome], to appear in 'Epioptics-7', World Scientific, ed. A. Cricienti. (Task C4).
  - **J304 (N)** ``Validity of effective-medium theory for optical properties of embedded nanocrystallites from ab initio supercell calculations", H.-Ch. Weissker [Jena], J. Furthmüller [Jena], F. Bechstedt [Jena], Phys. Rev. B **67**, 165322 (2003) (Task A5).
  - **L18 (N)** ``Basic density-functional theory - an overview", Ulf von Barth, Physica Scripta (Task D).
  - **R232 (N)** ``Calculation of optical properties within the Local Density Approximation to Density Functional Theory: application to Palladium", P. Monachesi [Rome], R. Capelli and R. Del Sole [Rome], The European Physical Journal B, **26**, 159, (2002) .
  - **S214 (N)** ``Electronic and Crystallographic Structure of Apatites", L. Calderin, M.J. Stott and A. Rubio [San Sebastián], Physical Review B **67**, 165420-1,9 (2003) (Task B1).
  - **S216 (N)** ``Laser-induced Control of (Multichannel) Intracluster Reactions: The Slowest is Always the Easiest to Take", A. González-Ureña, K. Gasmin, A. Rubio and P.M. Echenique, submitted (Task C1).

#### **Joint NANOPHASE publications Year 4 (1.6.03-31.5.04) added 19.10.04**

- **B250 (N\*)** ``Image resonance in the many-body density of states at a metal surface", G. Fratesi and G. P. Brivio and Patrick Rinke [Berlin] and R. W. Godby [York], Phys. Rev. B **68** 195404 (2003) (Task C2).

- **B401 (N\*)** ``Image States in Metal Clusters'', Patrick Rinke [Berlin], Kris Delaney [York], P. García-González [San Sebastián], and R.W. Godby [York], submitted (Task A3).
- **J300 (N\*)** ``Many-body and overlayer effects on surface optical properties'', F. Bechstedt [Jena], R. Del Sole [Rome], S. Glutsch, [Jena], P.H. Hahn [Jena], O. Pulci [Rome], W.G. Schmidt [Jena], *phys. stat. sol. (b)* **240**, 469 (2003) (Task C4).
- **J301 (N\*)** ``P-rich GaP(001)(2 × 1)/(2 × 2)surfaces: A hydrogen-adsorbate structure determined from first-principles calculations'', P.H. Hahn [Jena], W.G. Schmidt [Jena], F. Bechstedt [Jena], O. Pulci [Rome], R. Del Sole [Rome], *Phys. Rev. B* **68**, 033311 (2003) (Task C4).
- **L17 (N\*)** ``The Pd(100)  $\sqrt{5} \times \sqrt{5}$  R30° O surface oxide revised'', M. Todorova and E. Lundgren and V. Blum and A. Mikkelsen [NANOPHASE Postdoc Lund] and S. Gray and J. Gustafson and M. Borg and J. Rogal and K. Reuter and J. N. Andersen and M. Scheffler [Berlin], *Surface Science* **541**, 214 (2003) (Task C).
- **L406 (N\*)** ``Kinetic hindrance during the initial oxidation of Pd(100) at ambient pressures'', E. Lundgren, J. Gustafson, A. Mikkelsen [NANOPHASE postdoc Lund], A. Stierle, H. Dosch, M. Todorova J. Rogal K. Reuter and M. Scheffler [Berlin], *Phys. Rev. Lett.* **92**, 046101 (2004) (Task C).
- **P250 (N\*)** ``Long-range contribution to the exchange-correlation kernel of time-dependent density functional theory'', Silvana Botti [Paris], Francesco Sottile [Paris], Nathalie Vast [Paris], Valerio Olevano [Paris], H. Weissker [Jena], Lucia Reining [Paris], Angel Rubio [San Sebastián], Giovanni Onida [Rome], Rodolfo Del Sole [Rome] and R.W. Godby [York], *Phys. Rev. B* **69**, 155112 (2004) (Task A5,B4,C4).
- **P304 (N\*)** ``Optical and loss spectra of carbon nanotubes: Depolarization effects and intertube interactions'', **A.G. Marinopoulos [Paris: NANOPHASE-funded young researcher]**, Lucia Reining [Paris], Angel Rubio [San Sebastián], Nathalie Vast [Paris], *Phys. Rev. Lett.* **91**, 046402 (2003) (Task B4).
- **P306 (N\*)** ``Ab initio Study of the Optical Absorption and wavevector-dependent Dielectric Response of Graphite'', **A.G. Marinopoulos [Paris: NANOPHASE-funded young researcher]**, L. Reining [Paris], A. Rubio [San Sebastián], V. Olevano [Paris], *Phys. Rev. B* **69**, 245419 (2004) (Task B4).
- **P402 (N\*)** ``Density-Functional contributions to bandstructure calculations beyond the GW approximation'', F. Bruneval [Paris], F. Sottile [Paris], V. Olevano [Paris], N. Vast [Paris], L. Reining [Paris], R. Del Sole [Rome], *Phys. Rev. Lett.* (in preparation) (Task A3,B2,C1).
- **P403 (N\*)** ``Ab initio study of the wavevector-dependent dielectric response of solids of single-walled carbon nanotubes'', **A.G. Marinopoulos [Paris: NANOPHASE-funded young researcher]**, L. Reining [Paris] and A. Rubio [San Sebastián], *Phys. Rev. B* (in preparation) (Task B1,B4).
- **P404 (N\*)** ``A brief introduction to the ABINIT software package'', X. Gonze, G.-M. Rignanese, M. Verstraete, J.-M. Beuken, Y. Pouillon, R. Caracas, F. Jollet, M. Torrent, G. Zerah, M. Mikami, P. Ghosez, J.-Y. Raty, V. Olevano [Paris], F. Bruneval [Paris], L. Reining [Paris], R. Godby [York], G. Onida [Rome], et. al., *Zeitschrift fuer Kristallographie*, special issue "computational crystallography" (invited, submitted) (Task A3,A4,A5,B2,B4,C1,C2).

- **R299 (N\*)** ``Ab-initio calculation of the exchange-correlation kernel in solids'', G. Adragna, R. Del Sole [Rome], A. Marini [San Sebastian:NANOPHASE-funded Young Researcher], Phys. Rev. B 68, 165108 (2003) (Task A5).
- **R304 (N\*)** ``Optical anisotropy induced by cesium adsorption on the As-rich  $c(2 \times 8)$  reconstruction of GaAs(001)'', **C. Hogan** [Rome:NANOPHASE-funded Young Researcher], D. Paget, O.E. Tereschenko, L. Reining [Paris], and G. Onida [Rome], Phys. Rev. B 69, 125332 (2004) (Task C4).
- **R309 (N\*)** ``Many-body effects on the EEL spectrum of the C(100) surface'', M. Palummo [Rome], O. Pulci [Rome], **A. Marini, San Sebastian, network-funded young researcher**, R. Del Sole [Rome], V. Olevano [Paris], L. Reining [Paris], in preparation (Task C4).
- **R314 (N\*)** ``Early stages of cesium adsorption on the As-rich  $c(2 \times 8)$  reconstruction of GaAs(001): Adsorption sites and Cs-induced chemical bonds'', **C. Hogan [Rome: NANOPHASE-funded Young Researcher]**, D.Paget, Y.Garreau, M.Sauvage, G.Onida [Rome] L.Reining [Paris], P.Chiaradia, V. Corradini, Phys. Rev. B 68, 205313 (2003) (Task C4).
- **R401 (N\*)** ``Dynamical excitonic effects in metals and semiconductors'', **A. Marini [San Sebastián Nanophase Young Researcher]** and R. Del Sole [Rome], Phys. Rev. Lett. 91, 176402 (2003) (Task B4).
- **R407 (N\*)** ``Reflectance anisotropy spectra of the diamond (100) $2 \times 1$  surface: evidence of strongly bound surface state excitons'', M. Palummo [Rome], O. Pulci [Rome], R. Del Sole [Rome], **A. Marini, Nanophase Funded Young Researcher in San Sebastian**, M. Schwitters, S. R. Haines, K. H. Williams, D. S. Martin, P. Weightman, J. E. Butler, submitted (Task C4).
- **R409 (N\*)** ``The Bethe-Salpeter equation: a first-principles approach for calculating surface optical spectra'', M. Palummo [Rome], O. Pulci [Rome], R. Del Sole [Rome], **A. Marini, Nanophase funded young researcher in San sebastian**, P. Hahn [Jena], W. G. Schmidt [Jena], F. Bechstedt [Jena], J. of Phys. Condensed Matter, accepted (Task C4).
- **R414 (N\*)** ``Electronic structure of the C(111) surface: an ab-initio study'', M. Marsili [Rome], O. Pulci [Rome], F. Bechstedt [Jena], R. Del Sole [Rome], in preparation (Task C4).
- **R415 (N\*)** ``Electronic and optical properties of Ge nanowires beyond the one-particle approach'', M. Bruno [Rome], M. Palummo [Rome], R. Del Sole [Rome], V. Olevano [Paris, S. Ossicini, in preparation (Task B2, B4).
- **S220 (N\*)** ``Bound excitons in time-dependent density-functional-theory: optical and energy-loss spectra'', **A. Marini [San Sebastián Nanophase Young Researcher]**, A. Rubio [San Sebastián] and R. Del Sole [Rome], Physical Review Letters **91**, 256402-1,4 (2003) (Task B4).
- **S400 (N\*)** ``Optical absorption and electron energy loss spectra of carbon and boron nitride nanotubes: a first principles approach'', **A.G. Marinopoulos [Paris Nanophase Young Researcher]** L. Wirtz [San Sebastián], **A. Marini [San Sebastián Nanophase Young Researcher]**, V. Olevano[Paris], A. Rubio[San Sebastián] and L. Reining [Paris], Applied Physics A **78** 1157-1167 (2004) (Task B4).
- **S411 (N\*)** ``Assessment of Density Functional Approximations: Long-Range

- Correlations and Self-Interaction Effects", J. Jung, P. García-González [San Sebastián], J.E. Alvarillos and R. W. Godby [York], Phys. Rev. A **69** 052501 (2004) (7 pages) (Task A3).
- **S412 (N\*)** ``Effects beyond the RPA in the interaction between metal films'', J. Jung, P. García-González [San Sebastián], J. F. Dobson and R. W. Godby [York], submitted (Task A2).
  - **Y401 (N\*)** ``Comment on `Band-Gap Problem in Semiconductors Revisited: Effects of Core States and Many-Body Self-Consistency'', Kris Delaney [York], P. García-González [San Sebastián], Angel Rubio [San Sebastián], Patrick Rinke [Berlin] and R.W. Godby [York], submitted (Task A2).

### **Other NANOPHASE publications Year 4 (1.6.03-31.5.04) added 19.10.04**

- **S402 (N)** ``Excited states dynamics in time-dependent density functional theory: high-field molecular dissociation and harmonic generation'', A. Castro, **M.A.L. Marques**[San Sebastián Nanophase Young Researcher], J.A Alonso, G.F. Bertsch, y A. Rubio[San Sebastián], European Journal of Physics D **28** 211-218 (2004) (Task A3).
- **S403 (N)** ``Electrical transport in carbon nanotubes: role of disorder and helical symmetries'', F. Triozon, S. Roche, A. Rubio [San Sebastián] and D. Mayou, Physical Review B (Rapid Communications) **69** R121414-1,4 (2004) (Task B3).
- **S410 (N)** ``Theoretical identification of Stone-Wales defects in nanotubes'', Y. Miyamoto, A. Rubio [San Sebastián], S. Berber, M. Yoon, and D. Tománek, Physical Review B (Rapid Communications) **69** R121413-1,4 (2004) (Task B2).
- **B251 (N)** ``Ab initio study of the half-metal to metal transition in magnetite'', **M. Friák** [Berlin: NANOPHASE-funded Young Researcher], A. Schindlmayr [Berlin] and M. Scheffler [Berlin], submitted (Task A5).
- **J307 (N)** ``Quasiparticle band structures and optical spectra of  $\beta$ -cristobalite SiO<sub>2</sub>'', L.E. Ramos [Jena: NANOPHASE-funded Young Researcher], J. Furthmüller [Jena], F. Bechstedt [Jena], Phys. Rev. B **69**, 085102 (2004) (Task A5).
- **J400 (N)** ``Quantum structures in SiC'', F. Bechstedt [Jena], A. Fissel, J. Furthmüller [Jena], U. Kaiser, H.-Ch. Weissker [Jena], W. Wesch,, Appl. Surf. Sci. **212-123**, 820 (2003) (Task A5).
- **J401 (N)** ``Excitation energies and radiative lifetime of Ge<sub>1-x</sub>Si<sub>x</sub> nanocrystals: Alloying versus confinement effects'', H.-Ch. Weissker [Jena], J. Furthmüller [Jena], F. Bechstedt [Jena], Phys. Rev. Lett. **90**, 085501 (2003) (Task A4).
- **J402 (N)** ``Excitonic and local-field effects in optical spectra from real-space time-domain calculations'', W.G. Schmidt [Jena], P.H. Hahn [Jena], F. Bechstedt [Jena], High Performance Computing in Science and Engineering '02, ed. by E. Krause, W. Jäger, (Springer, Berlin 2003) p. 133 (Task C4).
- **J403 (N)** ``The InP(001)(2 × 1)surface: A hydrogen-stabilized structure'', W.G. Schmidt [Jena], P.H. Hahn [Jena], F. Bechstedt [Jena], N. Esser, P. Voigt, A. Wange, W. Richter, Phys. Rev. Lett. **90**, 126101 (2003) (Task C2, C4).
- **J404 (N)** ``Optical response of semiconductor surfaces and molecules calculated from first principles'', W.G. Schmidt [Jena], M. Preuß[Jena], P.H. Hahn [Jena], K.

- Seino [Jena], F. Bechstedt [Jena], High Performance Computing in Science and Engineering, Munich 2002 (Springer, Berlin 2003), p. 259 (Task C2, C4).
- **J405 (N)** ``Tetramers on diamond'', Si and Ge(113) surfaces: Ab initio studies, A.A. Stekolnikov [Jena], J. Furthmüller [Jena], F. Bechstedt [Jena], Phys. Rev. B **68**, 205306 (2003) (Task C4).
  - **J406 (N)** ``Layer-by-layer analysis of surface reflectance anisotropy'', C. Castillo, B.S. Mendoza, W.G. Schmidt [Jena], P.H. Hahn [Jena], F. Bechstedt [Jena], Phys. Rev. B **68**, 041310(R) (2003) (Task C4).
  - **J407 (N)** ``Vibrational properties of the quasi-one-dimensional In/Si(111)(4 × 1) system'', F. Bechstedt [Jena], A. Krivosheeva, J. Furthmüller [Jena], A.A. Stekolnikov [Jena], Phys. Rev. B **68**, 193406 (2003) (Task C4).
  - **J408 (N)** ``Influence of structural relaxation on the optical and electronic properties of Ge and Si nanocrystals'', H.-Ch. Weissker [Jena], J. Furthmüller [Jena], F. Bechstedt [Jena], Proc. Int. Symp. Clusters and Nano-Assemblies: Physical and Biological Systems, Richmond (USA) 2003 (Task A5).
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