CURRICULUM VITÆ of

Stefano de GIRONCOLI,

born in Trieste (Italy), [redacted], two children.

Present position

Full Professor at the
International School for Advanced Studies (ISAS) –
Scuola Internazionale Superiore di Studi Avanzati (SISSA)
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Education

1983-1988	Undergraduate studies in Physics at the *Università di Trieste*, Trieste (Italy).
October 1st 1988	Degree in Physics at the *Università di Trieste*, Trieste (Italy), with a thesis on "Piezoelectric properties of III-V binary semiconductors" (in italian) under the supervision of Prof. A. Baldereschi
1989-1992	Ph.D. studies at the *Institut Romand de Recherche numérique en physique de MAtériaux (IRRMA)*, Lausanne (Switzerland).
October 29th 1992	Ph.D. degree (*docteur és science*) from the *Ecole Polytechnique Fédérale de Lausanne (EPFL)*, Lausanne (Switzerland), with a thesis on "ab-initio numerical studies in semiconductor alloys", under the supervision of prof. A. Baldereschi.

Teaching Activity

1989-92	Teaching assistant ("Electronic Properties of Solids") at the Physics Department of the /sl Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne (Switzerland).
1994-96	Lecturer on "Symmetries, electron bands and phonons" for the Diploma Programme of the *International Centre for Theoretical Physics (ICTP)*, Trieste (Italy).
1996–present	Lecturer on "Electronic structure" for the Ph.D. curriculum in Condensed Matter at SISSA.
2002–2006	Lecturer on "Quantum Mechanics" for the "Computational Physics" Master curriculum at the *Università di Udine*.
2009–present	Lecturer on "Electronic structure" for the diploma curriculum in Condensed Matter Physisc at ICTP.

1994–present

Supervisor of the Ph.D. work of
Michele Lazzeri (PhD: SISSA, 1999),
Matteo Cococcioni (PhD: SISSA, 2002),
Guido Fratesi (PhD: SISSA, 2005),
Paola Gava (PhD: SISSA, 2007),
Viet-Huy Nguyen (PhD: SISSA, 2008),
Lorenzo Paulatto (PhD: SISSA, 2009).
Currently supervising the Ph.D. work of Ngoc-Linh Nguyen, Emine Küçükbenli, Riccardo Sabatini.
Co-supervisor, with Stefano Baroni, of the Ph.D. work of the following students:
Claudia Bungaro (PhD: SISSA, October 1995),
Antonino Marco Saitta (PhD: SISSA, October 1997),
Gabriele Cipriani (PhD: SISSA, October 2000).
Co-supervisor, with Alessandro Baraldi of the Ph.D. work of Laura Bianchettin (UniTS, 2008).
Co-supervisor, with Giovanni B. Bachelet, of the Diploma work of Alessandra Iacobucci (Università "la Sapienza", Roma (Italy), 1997).

Research Activity

My research activity aims at the understanding of the properties of materials (insulators, semiconductors, and metals including their surfaces, alloys, and defects), starting from a first-principles quantum (Density Functional Theory) description of their microscopic constituents –electrons and nuclei– i.e. of the chemical bond between atoms. My research activity is mainly computational in nature and it involves the development of original and efficient methods to deal with the numerical challenges posed by the *ab initio* modeling of realistic systems.
Sometime this requires the development of original algorithms and methods of calculation, as it is the case for the development of Density Functional Perturbation Theory (DFPT)—a general method to calculate efficiently electronic response functions in solids—that have been developed in our group and to which I have contributed in several ways. Often it involves the invention of approximate approaches and their validation for the *particular* systems under study, as it is the case for the so-called *computational alchemy* approach to the thermodynamics of substitutional alloys, that I have developed.

Stefano de Gironcoli's current research interests include

- van der Waals interaction in DFT:
Ubiquitus van der Waals interactions pose a severe challenge to the currentlly widespread LDA and GGA exchange and correlation functionals in DFT. In fact the intrinsically non-local correlations responsible for these effects cannnot be accounted for by ANY semilocal functional. The Adiabatic-Connection Fluctuation-Dissipation (ACFD) formalism offer an in principle exact way to address the problem but its use is hampered by a extremely heavy computationl cost. We are working hard to develop efficient and accurate numerical methods to calculate the RPA correlation energy within the ACFD formalism via eigenvalue decomposition of the imaginary frequency dependent response function of the system. Starting from the exact ACFD formula, approximate functionals have been proposed by Langreth and co-workers that are expected to describe the effects van der Waals interaction. Comparison of the different approaches will help benchmerking and improving the accuracy of this new class of XC functinals.

- Reactivity at surfaces:
In the past years adsorption of simple molecules on transition metal surfaces has been studied expensively. More recently the reactivity of metallic surfaces toward methane dehydrogenation has been studied and it has been shown, for instance, that a model catalyst formed by a single Rh adatom on Rh(111) surface is able, if operated at low enough temperature, to effectively induce the first deprotonation while hindering the second one, thus preventing poisoning and coking. Model mechanisms for low temperature methane-to-methanol conversion, avoiding the two high-temperature steps involved in the industrial process, have also been studied. Other reactions that are being studied are the partial oxidation of Ethylene to Etylene Epoxide on metallic nanoparticles and the syntesis of Ammonia on small Iron Sulfur clusters.

- Theoretical core level spectroscopy :
A fruitful collaboration has been established with A.Baraldi and coworkers at the Elettra superESCA beamline to analyze, with a combined experimental (XPS) and theoretical (DFT) approach, the effect of local chemical and geometrical environment on core-level binding energy shifts of surface atoms and adsorbates. The possibility to identify and monitor the presence of low coordination defects, such as isolated Rh adatom or dimers on a clean Rh (001) surface, has been demonstrated. Local changes in the electronic structure induced on the metallic surface by adsorbed species, such as nitrogen, carbon and sulfur, are now under investigation. The collaboration has strengthened even more with the involvement of L. Bianchettin, a PhD student at Trieste University, that worked both on the experimental and theoretical aspects of the problem.

- LDA+U method :
Traditional methods in DFT (LDA and GGA approximations) in spite of their many successes fail badly in certain cases. Beside the van der Waals interaction problem that will be addressed later, one of the most spectacular failure of LDA/GGA approaches is the incorrect metallic description of many transition metal or rare earth oxides, while they are Mott-type insulators experimentally. LDA+U approach, first introduced by Anisimov and coworkers in the '90, has allowed to study a large variety of strongly correlated compounds with considerable improvement with respect to LSDA or $\sigma-$GGA results. Weak points in LDA+U methodology are the fact that it is usually formulated assuming a localized atomic-like basis set for the wavefunction expansion and the often semiempirical determination of the relevant parameter U. In collaboration with With M.Cococcioni I have readdressed the problem by defining the LDA+U correction in terms of general projectors and devising an internally consistent way to compute U from first-principles.

- Cerium Oxydes :
Highly-active catalysts are based on metal nano-particles (Au, Pt, Rh, Pd) supported by reducible metal oxides, such as cerium oxides (ceria). The mechanisms responsible for the superior catalytic activity of these devices rely on electronic effects following the creation of oxygen vacancies which in turn are associated to the presence of strongly correlated f-electrons in Ce. Our previous work on LDA+U opened the way to the first-principles study of ceria and a first result has been the realistic description of electronic and structural properties of oxygen vacancies in bulk ceria. This work has been done in collaboration with S.Baroni, S.Fabris, G. Balducci and one of his PhD students. The collaboration is continuing with the study of hydrogen adsorption on oxidized and reduced ceria surfaces and the corresponding vibrational signatures.

- High Pressure physics :
In collaboration with R.M. Wentzcovitch (U.Minnesota) and her coworkers I have studied the thermoelastic properties of candidate mineral phases in Earth's lower mantle, focusing so far on Fe-free phases. Iron content in lower mantle mineral phases is estimated to be 10-20 % but its theoretical treatment by LDA/GGA approximation is again problematic. Progress made on LDA+U implementation allows us now to attack the problem of iron incorporation in magnesium-wustite (MgFe)O and/or in iron-magnesium perovskite (MgFe)SiO3 and we are now addressing the problem of the High-Spin–Low-Spin phase transition observed experimentally in magnesium-wustite at pressure relevant for the Core-Mantle D" boundary layer.

- further software and theoretical developments :
In addition to the above, I'm very interested in methodological/theoretical developments and in their actual implementation in the computational engine that lies at the core of all the simulations we are performing or may wish to perform in the future, namely into the quantum-ESPRESSO package. In particular I'm deeply interested in developments that can enhance the overall accuracy of the calculations we can perform. In this context, I have coordinated the implementation of Bloechl's Projected Augmented Wave (PAW) formalism in Quantum-ESPRESSO. This effort will allow us, and the scientific community utilizing these codes, to perform all-electron calculations with the efficiency typical of a plane-wave pseudopotential approach.
Also, I'm working on the implementation of hybrid DFT-Hartree-Fock features in Quantum-ESPRESSO. Although considerably more computationally demanding than traditional LDA or GGA formulations, hybrid functionals (B3LYP, PBE0, ...) appears to be more predictive in a number of thermochemistry calculations. Moreover, any further attempt to model more accurately the correlation part of the XC functional could be spoiled by a poor treatment of the exchange part.

Stefano de Gironcoli's past research achievements:

- Piezoelectric Constants of semiconductors: (A1, A3)
I have developed the DFPT formulation for the calculation of piezoelectric properties of materials. This has allowed the first theoretical determination of piezoelectric constant in III-V and II-VI zincblend semiconductors, and has shown that the accuracy that can be obtained for these properties is similar to the one that can be obtained for other response functions to macroscopic electric fields such as the dielectric constants and the Born effective charges.
- Thermodynamics of substitutional alloys: (A5, A14, A24, A34)
I have developed an original approach for the study of the thermodynamical properties of substitutional alloys, based on a perturbative (via DFPT) expansion of the configurational energy of the alloy, truncated to second order and supplemented, when needed, with a cluster expansion of the residual energy-error. This allows to map the energetics of the alloy upon a Ising-like model that is hence studied via MonteCarlo simulations. A few cases of semiconductor alloys have been studied with this approach.
- Vibrational properties: (A4, A11, A17, A18, A19, A20, A25, A41, A43)
I have generalized the original formulation of DFPT, applied to the study of vibrational properties, to perturbations of any periodicity, thus allowing the efficient calculation of full phonon dispersions in solids. Later, I have generalized DFPT to the study of metallic systems. This formulation preserves the elegance of the original approach also in the case of gapless materials and has been the basis for the subsequent activity of the group on vibrational properties of metallic surfaces. More recently, I contributed to the spin polarized extension of DFPT.
Sometime the vibrational properties of a given system are interesting by themselves, but often the knowledge of its vibrational properties is the fundamental intermediate ingredient needed for the computation of other interesting properties as it is discussed in the following points.

- Vibrational properties of semiconductor alloys and superlattices: (A2, A6, A7, A8, A9, A10, A12, A13, A15, A16, A38)
Vibrational properties are used to experimentally monitor the perfectness of semiconductor superstructure. This requires however reliable knowledge of the vibrational properties as a function of the structural details.
In the case of GaAs-AlAs alloys and superlattices, a *lattice matched* semiconductor system, we showed that the chemical difference between the two cations is so small that a very accurate description of their vibrational properties can be obtained by taking into account the mass difference between the two cations and considering a unique (average) set of interatomic force constants for both materials (*mass approximations*). In this way very detailed results have been obtained for the homogeneous alloy, and for ideal and partially interface-intermixed superlattices.
If very accurate results are desired, the mass approximation cannot be used directly when the chemical difference or the lattice mismatch between constituents are large. For this reasons I have introduced later some corrections to it in terms of higher-order interatomic force constants (HIFC). In this way also the vibrational properties of Si-Ge systems were described with very good accuracy.
Later, in collaboration with C. Bungaro, I studied the vibrational properties of $Al_xGa_{1-x}N$ homogeneous alloys. In this case, the chemical similarity between cations is such that, in spite of the lattice mismatch between the two alloy end-members, the mass approximation is satisfied within a few percent. This allowed us to determine the nature of the zone-center vibrations in this alloy that appears to be a mixed one-mode two-mode system, with vibrations of some symmetry displaying a clear one-mode behavior, and those of other symmetries displaying two-mode behavior.

- Temperature effects in bulk materials and their surfaces within the Quasi Harmonic Approximation: (A23, A26, A28, A29, A30, A35, A36, A39, A44, A45)
The inclusion of the effects of temperature in the description of a given physical system is a difficult task that could require very detailed molecular dynamics studies or some approximate treatment of the anharmonic terms in the interatomic potential.
The knowledge of the vibrational properties of a system, in a given structural configuration, allows to approximately calculate its free energy. Their dependence as a function of the structural parameters allows to study its temperature behavior within the so called Quasi Harmonic Approximation (QHA). This approximation is expected to be accurate as long as the temperature is not too close to the melting point, but no much experience in this respect is presently available.
In collaboration with R. Wentzcovitch *et al.*, I have studied, using QHA, the High-T, High-P equation of state and elastic constants of MgO and $MgSiO_3$, that are believed to be, alloyed with Fe, among the major constituents of the Earth lower mantle. In all these cases, QHA appears to work well in the range of temperature of interest.

- Thermal expansion of surfaces

I have studied the thermal expansion of some bulk metals and their surfaces. In particular, with my student M. Lazzeri, I studied very carefully the thermal expansion of Be (0001) surface that displays experimentally a large thermal expansion of the first surface layer. In this specific case we thoroughly checked the validity of QHA with respect to a full first-principle molecular dynamics (FPMD) simulation at 700 K and the two schemes were essentially equivalent for the temperature considered. Surprisingly enough, both QHA and FPMD calculations showed a much smaller surface thermal expansion than experimentally observed. In order to understand this discrepancy, I'm collaborating with an experimental group that is performing an independent determination of the surface thermal expansion in Be (0001), by the study of the temperature dependence of the surface core level shifts (SCLS), to be compared with a theoretical calculation of SCLS as a function of surface relaxation.

In order to be able to study thermal expansion of more complex surfaces, characterized by several structural parameters, the efficient calculation of the derivative of the vibrational frequencies w.r.t. atomic positions, i.e. the calculation of third order derivatives of the total energy, is needed. We have developed a computer code for the calculation of these derivatives. This required the nontrivial extension of the so-called "2N+1 theorem" to metallic systems. This approach has then be applied to Be and Mg $(10\bar{1}0)$ surfaces.

Invited Talks to International Conferences

I47) SIF 99 congress: Trieste, September 23-29, 2013 Lecture Title: "Nonlocal van der Waals Density Functional made simple and efficient"

I46) What about U ? June 2012 Kenya. CECAM workshop on "What about U? - Corrective approaches to DFT for strongly-correlated systems." Lausanne, Switzerland, June 18 to 21, 2012 Title: "Correlation energy from Adiabatic Coupling Fluctuation-Dissipation."

I45) ASESMA 2112: African School on Electronic Structure Methods and Applications, June 2012 Kenya..

I44) National Magnetic Resonace Society conference on "New Developments in NMR", February 5-8, 2012, Bangalore, Lecture Title: "Complete 13C Chemical Shift assignment For Cholesterol Crystal by combined CP-MAS Spectral Editing and ab-initio GIPAW Calculations"

I43) ETSF conferencer 2011 "Bridging Theory and Experiment", 26-30 September 2011, Torino, Lecture Title: "NMR with Density Functional Perturbation Theory"

I42) Workshop "São Paulo Advanced School on Computational Material Science for Energy and Environment Applications", 5-16 September 2011, UFABC Santo Andre, Brazil. Several lectures and QE tutorials
I41) Satellite Meeting "Theoretical Modelling of Materials" of the "9^{th} World Congress of the World Association of Theoretical and Computational Chemists (WATOC)", 13-15 July, Barcelona (Spain) Keynote Lecture Title: "Reactivity at metal and metal oxide surfaces"

I40) Workshop "Structural Predictions using USPEX", 27-30 June 2011, ENSIP-Poitiers, Poitiers University, France. Lecture Title: "Surfaces"

I39) Workshop "Periodic DFT for Beginners", 23-25 June 2011, ENSIP-Poitiers, Poitiers University, France. Lectures Title: "Introduction to the Quantum Espresso code" and "LDA and the other approaches. Successes and Failures"

I38) Indian Institute for Scientific Education and Research (IISER), Pune, November 23, 2010. Title: "What determines Catalyst's Selectivity in the Ethylene Epoxidation Reaction ?"

I37) CECAM workshop on "van der Waals forces in DFT, RPA and beyond" Lausanne, Switzerland, June 28 to July 2, 2010 Title: "Efficient and accurate calculation of exact exchange and RPA correlation energies in ACFD theory

I36) CECAM workshop on "Electronic-structure challenges in materials modeling for energy applications" Lausanne, Switzerland, June 1-4, 2010. Title: "Efficient and accurate calculation of exact exchange and RPA correlation energies in ACFD theory

I35) Soirée "van der Waals Forces", Thomas Young Center, King's College, London (UK), June 18 2009. Title: "Efficient and accurate calculation of exact exchange and RPA correlation energies in ACFD theory"

I34) A*star Intitute for High Performance Computing, Singapore, March 27 2009.

I33) JNCASR, Bangalore, March 24 2009.

I32) CECAM-Psi-k Workshop on "Mineral spectroscopy by theory and experiment", Lausanne, Switzerland, October 6-9, 2008. Title: "Going beyond Local Density and Gradient Corrected XC functionals in Quantum-ESPRESSO"

I31) East African School in Computational and Materials Science , Addis Ababa, Ethiopia, 15-26 September 2008

I30) S.Barbara 2008 Title: "van der Waals interaction in DFT"

I29) School on Electronic Structure Methods, AIMS, Cape Town, South Africa, 14-25 July 2008

I28) Americal Chemical Society, Boston 19-23 August 2007, Title: "Modelling reactivity of metal catalysts: methane activation, Methanol synthesis, Ethylene epoxidation"

I27) XIII International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, 11-13 January 2007, Trieste (Italy).
Title: "van der Waals interaction in DFT: a simple approximation for the polarizability"

I26) International Conference on Quantum Simulators and Design, December 3-6, 2006 Hiroshima University, Higashi-Hiroshima Campus.
Title: "Engineering the reactivity of metal catalysts: low temperature methanol synthesis"

I25) Italian-Swiss workshop on *high-performance computating in material science*, 21 - 23 September 2006, Cala di Lepre, Palau (SS), Italy
Title: "Theoretical Heterogeneous catalysis for Energy Applications".

I24) Bangalore Summer School on "Electronic Structure Methods and their Applications" in conjunction with Conference on Computational Materials Theory, 10 - 22 July 2006, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India
Title: "Engineering the reactivity of metal catalysts: low temperature methanol"

I23) American Physical Society 2006 March Meeting, 13 - 17 March 2006, Baltimore, MD (USA)
Title: "Electronic Structure and Phase Tranmsitions in Iron bearing Minerals"

I22) First VLab workshop, 20 July - 23 July, Minneapolis (USA).
Title: "Going beyond Local Density and Gradient Corrected XC functionals in Quantum-espresso"

I21) ICTP School On Electronic-Structure Calculations And Their Applications in Materials Science, 25 April - 6 May 2005. Isfahan (Iran).
Title: "Ceria as an active Catalytic substrate: Mixed valency in Density Functional Theory"

I20) ICTP-NSFC-ICTS Asian/Pacific Regional Schools on "Electronic Structure Methods and Their Applications" 19-30 July 2004, Beijing (China).
Title: " Mixed valency in Density Functional Theory The case of (defective) ceria".

I19) Electronic Structure Conference , May 2003, Minneapolis, Minnesota (USA).
Title: "LDA+U calculations of Iron Containing Minerals".

I18) 10th International Workshop on Computational Material Science: Electronic Structure Theory and Simulations, January 2003, Trieste (Italy).
Title: "LDA+U calculations of Iron Containing Minerals".

I17) CECAM workshop on *"Ab-initio Theoretical Approaches to the Electronic Structure and Optical Spectra of Materials"*, 23-25 September 2002, Lyon, France.
Title: "Vibrational broadening of core-level excitations from first principles".

I16) Materials Research Society, Spring 2002 Meeting April 1-5, San Francisco, California (U.S.A.).
Title: "High-pressure thermoelasticity of perovskite minerals from first principles lattice dynamics".

I15) CECAM workshop on *"Future developments in the study of structure-property relations by computational crystallography and experiments"*, 23-27 October 2000, Lyon, France.
Title: "First principles lattice dynamics: application to high-pressure thermoelasticity of minerals".

I14) Spring Colleges on *"Computational Physics"*, May - June 2000, International Centre for Theoretical Physics (ICTP), Trieste (Italy). Two lectures on : "Ab-initio Electronic Structure calculations".

I13) International Workshop on Thermodynamics and Structural properties of Alloys Materials, 20 - 24 June 1999, Aruba.
Title:"Phase Diagrams and Electronic Structure of II-VI Alloys".

I12) 9th International Workshop on Computational Material Science: Electronic Structure Theory and Simulations, 14 - 16 January 1999, Trieste (Italy).
Title: "Ab-initio study of Be (0001) surface thermal expansion".

I11) 9th International Conference on Vibrations at Surfaces, 12 - 16 October 1998, Shonan Village Center, Hayama, Kanagawa-ken, Japan
Title:"Dynamical Properties of Solid Surfaces from Density-Functional Perturbation Theory".

I10) American Physical Society 1998 March Meeting, 16 - 20 March 1998, Los Angeles, california (U.S.A.)
Title:"Phase Diagrams and Electronic Structure of II-VI Alloys".

I9) International Workshop on *"Large-Scale Quantum Simulations: Total Energy and Force Methods"*, 12-14 January 1998, Tsukuba, Japan.
Title: "Ab-initio Dynamical Properties of Be (0001) surface".

I8) Spring Colleges on *"Computational Physics"*, 19 May - 27 June 1997, International Centre for Theoretical Physics (ICTP), Trieste (Italy).
5 Lezioni dal titolo: "Ab-initio Electronic Structure calculations".

I7) 16th European Conference on Surface Science, 9-13 Sep. 1996, Genova (Italy).
Title: "Ab-initio calculation of phonon spectra: theory and applications".

I6) VI Italian-Swiss workshop on *computational material science*, 28 Sep. - 2 Oct. 1996,
S. Margherita di Pula, Sardinia (Italy).
Title: "Ab-initio calculations in alloys".

I5) Workshop on *"ab-initio phonons"*,1-3 July 1996, Centre Européen de Calcul Atomique et Moléculaire (CECAM), Lyon (France).
Title: "Theory of the anomalous Rayleigh dispersion at H/W(110) surfaces".

I4) Workshop on *"Local Density and beyond"*, 17-28 June 1996, International Centre for Theoretical Physics (ICTP), Trieste (Italy).
Title: "LDA and LSD approximations".

I3) Fisrt workshop on *Vectorial and Parallel Computing of Electronic Properties of Solids*,
29-31 May 1991, Taormina (Messina, Italy).
Title:"Structure and Thermodynamics of Si_xGe_{1-x} Alloys from ab-initio Monte-Carlo Simulations".

I2) Fifth international workshop on *Computational Condensed Matter Physics: Total Energy and Force Methods*, 16-18 Jan. 1991, Trieste (Italy).
Title:"Structure and thermodynamics of Si_xGe_{1-x} alloys from ab-initio Monte-Carlo simulations".

I1) The 1990 Williamsburg workshop on *first-principles calculations for ferroelectrics*, 4-6 Feb. 1990, Williamsburg, Virginia (USA).
Title:"Piezoelectricity in III-V and II-VI semiconductors: a systematic ab-initio calculation".

Papers appeared on International Journals with peer-review
H-index = 36 (ISI web of knowledge, July 2015)

- A123 A. Rossi, S. Piccinin, V. Pellegrini, S. de Gironcoli, V. Tozzini,
  Nano-scale corrugation in Graphene: a density functional theory study of structure, electronic properties and hydrogenation,
  J. Phys. Chem. C **119**, 7900-7910 (2015).

- A122 G. Miceli, S. de Gironcoli, A. Pasquarello,
  Isobaric first-principles molecular dynamics of liquid water with nonlocal van der Waals interactions,
  J. Chem. Phys. **142**, 034501 (2015).

- A121 N. Colonna, M. Hellgren,S. de Girocoli,
  Correlation energy within the exact-exchange adiabatic connection fluctuation-dissipation theory: systematic development and simple approximations,
  Phys. Rev. B **90**, 125150 (2014).

- A120 N.L. Nguyen, N. Colonna, S. de Gironcoli,
  Ab-inito self-consistent total-energy calculations within the EXX/RPA formalism,
  Phys. Rev. B **90**, 045138 (2014).

- A119 B. Himmetoglu, A. Floris, S. de Gironcoli, M. Cococcioni,
  Hubbard-corrected DFT energy functionals: the LDA+U description of correlated systems,
  Int. J. Quantum Chem. **114**, 14-49 (2014).

- A118 B.I. Adetunji, G.A. Adebayo, S. de Gironcoli,
  Structural and elastic properties of strained $Mg_{1-x}Sr_xSe$ revealed,
  Solid State Commun. **178**, 46-49 (2014).

- A117 A.R. Ferreira, E. Kucukbenli, S. de Gironcoli, W.F. Souza, S.S.X. Chiaro, E. Kostantinova, A.A. leitao,
  Structural models of activated gamma-alumina surfaces revisited: thermodynamics, NMR and IR spectroscopies from ab-initio calculations,
  Chem. Phys. **423**, 62-72 (2013).

- A116 N.L. Nguyen, S. de Gironcoli, S. Piccinin,
  Ag-Cu catalysts for ethylene epoxidation: Selectivity and activity descriptors,
  J. Chem. Phys. **138**, 184707 (2013).

- A115 R. Sabatini, T. Gorni, S. de Gironcoli,
  Nonlocal van der Waals density functional made simple and efficient,
  Phys. Rev. B **87**, 041108 (2013).

- A114 R. Sabatini, E. Kucukbenli, B. Kolb, T. Thonhauser, S. de Gironcoli,
  Structural elolution of ammino acid crystals under stress from a non-empirical density functional,
  J. Phys. Cond. Matter **24**, 424209 (2012).

- A113) E. Kucukbenli, K. Sonkar, N. Sinha, S. de Gironcoli,
Complete C-13 NMR chemical shifts assignement for Cholesterol crystals by combined CP-MAS spectral editing and ab-initio GIPAW calculations with dispersion forces,
J. Phys. Chem. A **116**, 3765-3769 (2012).

  A112) A.R. Ferreira, E. Kucukbenli, A.A. Leitao, S. de Gironcloli,
Ab-initio Al-27 NMR chemical shifts and quadrupolar parameters for Al2O3 phases and their precursors,
Phys. Rev. B **84**, 235119 (2011).

- A111) A. Floris, S. de Gironcoli,E.K.U. Gross, M. Cococcioni,
Vibrational properties of MnO and NiO from DFT plus U-based density functional theory,
Phys. Rev. B **84**, 161102 (2011).

- A110) N.L. Nguyen, S. Piccinin, S. de Gironcoli,
Stability of intermediate States for Ethylene Epoxidation on Ag-Cu Alloy Catalysts: a first-principles investigation,
J. Phys. Chem. C **115**, 10073-10079 (2011).

- A109) N. Mammen, S. Narasimhan, S. de Gironcoli,
Tuning the morphology of gold cluster by substrate doping,
J. Am. Chem. Soc. **133**, 2801-2803 (2011).

- A108) A. Baraldi, L. Bianchettin, S. de Gironcoli, E. Vesselli, S. Lizzit, L. Petaccia, G. Comelli, R. Rosei,
Enhanced Chemical Reactivity of Under-Coordinated Atoms at Pt-Rh Bimetallic Surfaces: A Spectroscopic Characterization,
J. Phys. Chem. C **115** 3378-3384 (2011).

- A107) K. Umemoto, R.M. Wentzcovitch, S. de Gironcoli, S. Baroni,
Order-disorder phase boundary between ice VII and VIII obtained by first principles,
Chem. Phys. Letters **499**, 236-240 (2010).

- A106) P. Ghosh, R. Pushpa, S. de Gironcoli, S. Narasimhan,
Effective coordination number: A simple indicator of activation energies for NO dissociation on Rh(100) surfaces,
Phys. Rev. B **80**, 233406 (2009).

- A105) P. Giannozzi, et al.
QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials,
J. Phys. Cond. Matt. **21**, 395502 (2009).

- A104) Z. Wu, J.F. Justo, C.R.S. da Silva, S. de Gironcoli, R.M. Wentzcovitch,
Anomalous thermodynamic properties in ferropericlase throughout its spin crossover transition,
Phys. Rev. B **80**, 014409 (2009).

- A103) L. Bianchettin, A. Baraldi, S. de Gironcoli S, E. Vesselli, S. Lizzit, G. Comelli, and R. Rosei,
Surface Core Level Shift: High Sensitive Probe to Oxygen-Induced Reconstruction of Rh(100),
J. Phys. Chem. C **113**, 13192-13198 (2009)

- A102) H.-V. Nguyen, and S. de Gironcoli,
Efficient calculation of exact exchange and RPA correlation energies in the adiabatic-connection fluctuation-dissipation theory,
Phys. Rev. B **79**, 205114 (2009).

- A101) R. Pushpa, P. Ghosh,Prasenjit, S. Narasimhan, and S. de Gironcoli,
Effective coordination as a predictor of adsorption energies: A model study of NO on Rh(100) and Rh/MgO(100) surfaces,
Phys. Rev. B **79**, 165406 (2009).

- A100) H.-V. Nguyen, and S. de Gironcoli,
Van der Waals coefficients of atoms and molecules from a simple approximation for the polarizability,
Phys. Rev. B **79**, 115105 (2009).

- A99) P. Gava, A. Kokalj, S. de Gironcoli, and S. Baroni,
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