FINAL REPORT ON THE Psi-k TUTORIAL

Efficient density-functional calculations with atomic orbitals: a hands-on tutorial on the SIESTA code.

University of Cantabria, Santander, Spain

June 7th-10th 2010

Organized by

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Abstract.

This was a four-day hands-on tutorial on the use of the SIESTA code (http://www.icmab.es/siesta), aimed at researchers from different disciplines who already use, or plan to use, SIESTA in their work and who would like to go beyond simply managing the code, to better understand its essential foundations and to learn to which problems and how exactly the code can be most successfully applied. Aimed also at students, the tutorial also offered a brief introduction into density-functional theory in a more general frame, to put the SIESTA code in context.

Apart from the consideration of standard tasks implemented in most *ab-initio* codes, such as how to calculate the electronic (band) structure, perform structure (geometry) relaxation, calculate lattice vibrations or run molecular dynamics simulations, some specific SIESTA topics were covered, such as the generation and use of pseudopotentials, the construction of basis sets of strictly localized numerical atomic orbitals, the efficient computation of the matrix elements with linear scaling methods, the role and behaviour of the real-space grid manipulations, and the smart use of parallelization. Also post-processing and visualization tools, which are becoming essential, were taught during the tutorial.

The tutorial consisted of morning lectures followed in the afternoon by practical "hands-on" sessions. Some basic knowledge of quantum mechanics, solid-state physics, and statistical physics were assumed, along with basic knowledge of UNIX and Fortran programming.

Scientific summary.

Motivation

Electronic structure codes have become mature enough to be used by scientists not trained in the development of the methods themselves. This is a shift away from traditional practice, in which the know-how and the right to use the code was acquired through a long "internship" (a PhD thesis or a postdoc appointment) in one of the groups dedicated to method and code development. Nowadays most codes are distributed with very light licensing restrictions or for affordable fees. While this ease of access is in principle a good thing, it carries the risk of uncritical or poor use of the codes by untrained people. There is thus an increasing demand for training in the sensible use of these methods, with the goal that the prospective user understands the physical and main technical approximations behind a method and can assess its reliability and its usefulness for a particular problem.

In the past few years, the possibility of treating large systems with some first-principles electronic-structure methods has opened up new opportunities in many disciplines, and ever more people not familiar with *ab-initio* calculations are being attracted to these codes. In particular, the SIESTA program (http://www.icmab.es/siesta) has become quite popular and is increasingly being used by researchers in geosciences, biology, and engineering (apart from the "home base" of materials physics and chemistry). Currently there are more than 2500 registered users all over the world (almost 40 % of the licensees are located in Europe, mostly in ESF-member countries), and the paper describing the method [J. Phys.: Condens. Mat. **14**, 2745-2779 (2002)] has more than 2100 citations. SIESTA's efficiency stems from the use of strictly localized basis sets and from the implementation of linear-scaling algorithms which can be applied to suitable systems. A very important feature of the code is that its accuracy and cost can be tuned in a wide range, from quick exploratory calculations to highly accurate simulations matching the quality of plane-wave methods.

SIESTA is distributed freely to academics, and a special effort has been made over the years to train people in its use. Previous SIESTA schools [addressing specific communities in Barcelona (1999), Lyon (1999), Rio de Janeiro (2000), Cambridge (2002), Lyon (2003), Lyon(2007), Barcelona (2007), San Sebastián (2007), Barcelona (2009)] were very succesful, typically with more applicants than could be accommodated, and the demand for a new one is noticeable in the pace of new registrations and the postings to the program's mailing list.

That was the main reason why we proposed a four-day hands-on tutorial on the use of the SIESTA code, intended for researchers who want to use the code and need, apart from basic practice, a grounding on the capabilities of the method and the approximations used.

Aims

A first aim of the tutorial was to show the students the thread between fundamental laws of physics and the properties of atomic aggregates, and, in so doing, transmit the difficulty of the problem and the essence of the approximations along that thread. The main take-home knowledge was: (i) what can be computed, (ii) how to do it, (iii) how good the results can be, and (iv) how bad they can be if things are not done critically and carefully (even if *ab-initio*). Apart from the basics of density-functional theory, molecular dynamics simulation and geometry relaxation, which are common to most codes, the specific SIESTA topics covered were the generation and use of pseudopotentials, the construction of basis sets of strictly localized numerical atomic orbitals, localization issues for linear scaling both in the computation of the matrix elements and in the resolution of the hamiltonian, as well as more technical ones such as the influence of the real-space grid and parallelization. Also post-processing and visualization tools, which are becoming essential, were covered during the tutorial.

It was not the purpose of this school to train new method developers (even if this is a possible first step for it), but to train future users of these methods. It is always very important to educate future *ab-initio* users in the critical use of these codes. We taught them to control and assess the mains approximations involved (LDA/GGA, pseudopotentials, basis sets, localization for linear scaling) as well as the more technical ones.

Audience

The tutorial was addressed to young people who plan on using electronic structure methods in their research. Some fundamental knowledge of quantum mechanics was assumed, as well as basic statistical mechanics for the molecular dynamics part. Basic solid state physics background was not strictly required. The basics of these areas were covered quickly to establish the language. We have decided not to assume any previous *ab-initio* training, as our experience is that many prospective users are interested in self-contained courses. Experts in other electronic structure methods could still profit from most of the lectures of interest, even if the course was less intensive for them.

The course was very succesful from the point of view of the interest raised. The final number of attendees was of 24. We could not expand the numbers because of limitations in the confirmed finantial support. During the practical sessions, each student worked alone on a PC computer.

The origin of the students was also very varied, both geographical (14 different nationalities: Russia, Spain, Belgium, Chile, Argentina, Germany, United Kingdom, Uzbekistan, Poland, Mexico, France, Colombia, India, and China) and in terms of the scientific field.

A list of attendees follows in the corresponding Section below.

Format

The main scheme adopted was that of morning lectures followed by afternoon practical sessions. The lectures were split into: (1) Formal lectures in the early morning, giving the theoretical background and fundamental aspects of the physics and/or methodology of the calculations, and (2) practical lectures in the late morning, with more practicalities related to the implementation and the actual SIESTA usage, preparing for the afternoon session.

Documentation and bibliography

All the information related with the organization of the tutorial (including the programme, venue, accomodation, sponsors and even some touristic information) is accesible through: http://www.siesta.unican.es

The materials related to the course (talks and exercises) can be found in the Documentation section of the SIESTA web site (http://www.icmab.es/siesta).

The key references used in the tutorial were:

[1] J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón, and D. Sánchez-Portal. *The Siesta method for ab-initio order-N materials simulations*, J. Phys.: Condens. Matter **14**, 2745-2779 (2002)

[2] D. Sánchez-Portal, P. Ordejón, and E. Canadell. *Computing the properties of materials from first principles with Siesta*, Principles and applications of density functional theory in inorganic chemistry II: Structure and bonding **113**, 103-170 (2004)

[3] D. Sánchez-Portal, E. Artacho, P. Ordejón, and J. M. Soler. *Density-functional method for very large systems with LCAO basis set*, Int. J. Quantum Chem. **65**, 453-461 (1997)

[4] E. Artacho, D. Sánchez-Portal, P. Ordejón, A. García, and J. M. Soler. *Linear-scaling ab-initio calculations for large and complex systems.*, Phys. Stat. Sol. (b) **215**, 809-817 (1999)

[5] J. Junquera, O. Paz, D. Sánchez-Portal, and E. Artacho. *Numerical atomic orbitals for linear-scaling calculations*, Phys. Rev. B **64**, 235111 (2001)

[6] E. Anglada, J. M. Soler, J. Junquera, and E. Artacho. *Systematic generation of finite-range atomic basis sets for linear-scaling calculations*, Phys. Rev. B **66**, 205101 (2002)

[7] P. Ordejón, D. A. Drabold, M. P. Grumbach, and R. M. Martin. *Linear system-size scaling methods for electronic-structure calculations*, Phys. Rev. B **51**, 1456-1476 (1995)

[8] E. Artacho, E. Anglada, O. Diéguez, J. D. Gale, A. García, J. Junquera, R. M. Martin, P. Ordejón, J. M. Pruneda, D. Sánchez-Portal, and J. M. Soler. *The* SIESTA *method. Developments and applicability*, J. Phys.: Condens. Matter **20**, 064208 (2008)

[9] E. Artacho, J. D. Gale, A. García, J. Junquera, R. M. Martin, P. Ordejón, D. Sánchez-Portal, and J. M. Soler. *Electronic structure calculations within localized orbitals: the* SIESTA*method*, Handbook of materials modeling, Volume 1. Electronic Scale, edited by S. Yip (Springer 2005), Chapter 1.5, p. 1-15

together with the basic DFT references:

[10] R. M. Martin. *Electronic structure: Basic theory and practical methods*, (Cambridge University Press, Cambridge, UK, 2004)

[11] J. Kohanoff. *Electronic Structure Calculations for Solids and Molecules*, (Cambridge University Press, Cambridge, UK, 2006)

Lecturers

The lectures and practical sessions were conducted by members of the SIESTA development team and very experienced users. The detailed list of invited speakers and assistants for the practical sessions can be found at the corresponding Section.

Budget

Our purpouses were, at the very least, to cover the hotel, breakfast, lunch, and coffe break expenses of the participants, and the living and travel expenses of the speakers/presenters.

We got partial support from:

- The Psi-k network (5000 €).
- The University of Cantabria (2000 €).

We have asked also for support to the local Autonomous Government of Cantabria. We have not got any answer yet with the final figure we will be awarded (if any).

To close the budget, we were forced to ask for a fee of 275 € per student.

Conclusions and perspectives

The tutorial was very succesful both in attendance and satisfaction of the attendees. There is still considerable interest in learning the basic of *ab-initio* methods *f*or their use (this is a relatively new trend), and size-efficient methods are still very sought-after options. We do not see indications of decline of the interest of young scientists in these methods, which allows us to suggest some form of continuity. The success of this and previous courses is quite evident in view of the number of papers published using SIESTA and the number of citations of the main technical paper (over 2100, being the second most cited paper in the history of the review Journal of Physics: Condensed Matter).

Acknowledgments

We acknowledge the finantial support of the ESF Programme Psi-k, the University of Cantabria and the local Autonomous Government of Cantabria. We are indebted with the people of the Fundación Leonardo Torres Quevedo for their invaluable help in managing the Tutorials. We thank Esteban Stafford for his help with the computers setup.

Meeting program.

Day 1: June, 7th

8:30 Registration.
10:00 Welcome and practical issues. (Javier Junquera)
10:15 Introduction: Computer simulations and their role in research. (Alberto García)

11:00 Coffee break ————

11:30 Fundamentals: the quantum-mechanical many-electron problem and the Density Functional Theory approach. (Julian D. Gale)
12:15 Brief introduction to SIESTA. What is SIESTA good and efficient for?. Where does it stand in relation to other methods or codes?. (José Antonio Torres)
12:45 Introduction to the basic execution of SIESTA (input, output, tools, k-points, SCF...). (José Antonio Torres)

13:30 Lunch ——————

15:00 Practical session: first runs on simple examples. Basic visualization tools.

16:30 Coffee break ————

17:00 Practical session continued.

Day 2: June, 8th 2010

9:00 Pseudopotentials. General overview. (Alberto García)
9:45 Atomic orbitals of finite range as basis sets. (Javier Junquera)

10:30 Coffee break ————

11:00 How to generate and test pseudopotentials (including dealing with partial core corrections and semicore states). (Alberto García)
11:45 How to generate and test basis sets. (Javier Junquera)
12:30 How to generate variationally optimized basis sets. (Alberto García)

13:00 Lunch ————————

15:00 Practical session: How to generate smooth and transferable pseudopotentials. Converging the basis sets for realistic systems.

16:30 Coffee break ————

17:00 Practical session continued.

Day 3: June, 9h 2010

8:30 Brief introduction to the internal algorithms for computation of matrix elements and the electronic structure. (Javier Junquera)
9:15 Fundamentals on linear scaling. (Julian D. Gale)
10:00 Simulations of periodic systems. The sampling in reciprocal space. Computation of band structures in solids. (Andrei Postnikov)

10:45 Coffee break ————

11:10 The parallelization of SIESTA. (Julian Gale)
11:55 Simulation of magnetic systems: ferro and antiferromagnetic ordering. (Andrei Postnikov)
12:40 Systematic convergence for realistic projects: from quick and dirty to converged calculations. Filtering atomic orbitals to avoid the eggbox. (Daniel Sánchez-Portal)

13:10 Lunch ————————

15:00 Practical session: Systematic convergence for realistic problems.

16:30 Coffee break ————

17:00 Practical session continued.

Day 4: June, 10th 2010

8:30 Relaxations and geometry optimizations. (Alberto García)
9:15 Molecular Dynamics (MD) in different ensembles. (Julian Gale)
10:00 Calculations of vibrational spectrum and phonons. (Andrei Postnikov)

10:45 Coffee break ————

11:10 LDA+U: a primer and implementation in Siesta. (Daniel Sánchez-Portal)
11:55 Tools for the analysis of the electronic structure in relation to bonding properties. (Alberto García)
12:40 Practical code-handling matters: licences, updates and compilation. (José Antonio Torres)

13:10 Lunch ————————

15:00 Practical session: Computation of vibrational properties of materials. Molecular dynamic simulations on different ensembles. Beyond bare DFT simulations: the effect of correlation.

16:30 Coffee break ———

17:00 Practical session continued.

Curriculum vitae

Javier Junquera

Born in Córdoba (Spain) on 31 May 1974

Current appointment

Profesor Contratado Doctor-I3,
Departamento de Ciencias de la Tierra y Física de la Materia Condensada
Universidad de Cantabria
Avda. de los Castros s/n, E-39005, Santander, Spain
Tel: (+34) 942 20 15 16
FAX: (+34) 942 20 14 02
Email: javier.junquera@unican.es
web page: http://personales.unican.es/junqueraj

Research lines

First-principles calculations in Condensed-Matter Physics. Size effects on ferroelectric materials. Surface and interfaces phenomena. High-κ materials. Development of scientific computing codes.

Education

- Licenciado en Ciencias Físicas, Universidad de Oviedo, Spain (September 1996)

- Doctor en Ciencias Físicas, Universidad Autónoma de Madrid (advisors: P. Ordejón and E. Artacho) (September 2001)

Former appointments

- Sep 96-Mar 99
  PhD student, Departamento de Física,
  Universidad de Oviedo, Spain.

- Mar 99-Sep 99
  Profesor Asociado (Teaching Assistant), Departamento de Física de la Materia Condensada,
  Universidad Autónoma de Madrid, Spain.
- Sep 99-Sep 01
  Ayudante (Assistant Professor), Departamento de Física de la Materia Condensada,
  Universidad Autónoma de Madrid, Spain.
- Sep 01-Aug 03
  Assistant, Département de Physique,
  Université de Liège, Belgium.
- Aug 03-Sep 04
  Postdoctoral Associate, Department of Physics and Astronomy,
  Rutgers University, New Jersey, USA.
- Sep 04-Dec 08
  Ramón y Cajal Fellow
  Universidad de Cantabria, Spain.

Most relevant publications in the past ten years

1. J. Junquera, Ó. Paz, D. Sánchez-Portal, and E. Artacho, "Numerical atomic orbitals for linear-scaling calculations", Phys. Rev. B **64** 235111 (2001). Times cited: 249
2. J. M. Soler, E. Artacho, J. D. Gale, A. Garcia, J. Junquera, P. Ordejón, D. Sánchez-Portal, "The SIESTA method for ab initio order-N materials simulation", J. Phys.: Condens. Matter **14**, 2745-2779 (2002). Times cited: 2037
3. A. Anglada, J. M. Soler, J. Junquera, and E. Artacho, "Systematic generation of finite-range atomic basis sets for linear-scaling calculations", Phys. Rev. B **66** 205101 (2002). Times cited: 91
4. J. Junquera and Ph. Ghosez, "Critical thickness for ferroelectricity in perovskite ultrathin films" Nature **422**, 506-509 (2003). Times cited: 372
5. J. Junquera, M. Zimmer, P. Ordejón, and Ph. Ghosez, "First-principles calculation of the band offset at BaO/BaTiO3 and SrO/SrTiO3 interfaces" Phys. Rev. B **67**, 155327 (2003). Times cited: 34
6. C. Lichtensteiger, J.-M. Triscone, J. Junquera, and Ph. Ghosez, "Ferroelectricity and tetragonality in ultrathin PbTiO3 films", Phys. Rev. Lett. **94** 047603 (2005). Times cited: 86
7. "First-Principles Modeling of Ferroelectric Oxides Nanostructures", Ph. Ghosez and J. Junquera, in "Handbook of Theoretical and computational nanotechnology", Ed. by M. Rieth and W. Schoomers, (American Scientific Publisher, Stephenson Ranch, CA, USA, 2006). Review containing more than 100 pages, 61 figures, and 384 references. Times cited: 29
8. G. Geneste, E. Bousquet, J. Junquera, and Ph. Ghosez, "Finite-size effects in BaTiO3 nanowires" Appl. Phys. Lett. **88** 112906 (2006). Times cited: 33
9. V. Nagarajan, J. Junquera, J. Q. He, *et al.* "Scaling of structure and electrical properties in ultrathin epitaxial ferroelectric heterostructures" J. Appl. Phys. **100** 051609 (2006). Times cited: 22
10. P. Aguado-Puente, and J. Junquera " Ferromagneticlike closure domains in ferroelectric ultrathin films: first principles simulations." Phys. Rev. Lett. **100** 177601 (2008). Times cited: 13

Recent Invited Talks

1. "Ferroelectric properties of Ultrathin Perovskite Heterostructures" March Meeting of the American Physical Society (APS), Montreal (Canada), March 2004.

2. "A new proposal for a XML-based unified pseudopotential format", Twelfth International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, Trieste (Italy), January 2005.

3. "First-principles computations on size-effects in epitaxial ferroelectric heterostructures", 230th American Chemical Society (ACS) National Meeting, Washington DC (USA), August 2005.

4. "Interface effects in ferroelectric thin-film devices", Psi-k 2005 Conference, Swäbisch-Gmünd (Germany), September 2005.

5. "First-principles computations on size-effects in epitaxial ferroelectric heterostructures", Fall Meeting of the Material Research Society (MRS), Boston (USA), December 2005.

6. "A proposal for a unified norm-conserving pseudopotential format", Data representation and code interoperability for computational material physics and chemistry, Centre Européen of Calcul Atomique et Moléculaire, Lyon (France), April 2006.

7. "From 180° stripe domains to more exotic patterns of polarization in ferroelectric nanostructures", 31st International Symposium on dynamical properties of Solids, Porto (Portugal), September 2007.

8. "Ferromagnetic like closure domains in ferroelectric ultrathin films", Fundamental Physics of Ferroelectrics 2008, Colonial Williamsburg (Virginia, USA), February 2008.

9. "First-principles simulations of closure domains in ferroelectric ultrathin films", March Meeting of the American Physical Society (APS), Pittsburgh (PA, USA), March 2009.

10. "First-principles modeling of screening in ferroelectric ultrathin capacitors", Villa Conference on Complex Oxides Heterostructures, St. Thomas (Virgin Islands, USA), September 2009.

Organization of research activities

- Co-organizer of the SIESTA School (Linear-Scaling LCAO Program), "Linear-scaling ab initio molecular modelling of environmental processes" July 2002 (University of Cambridge, UK). 60 participants.
  (http://www.uam.es/siesta and follow the links to Tutorials).

- Lecturer in the "International Workshop in Computational Materials Science", May 2005 (Lanzhou, China).

- Organizer of the SIESTA Meeting, April 2006 (Santander, Spain).

- Organizer of the MOLSIMU Tutorial: "Efficient density functional calculations with atomic orbitals: a hands-on tutorial on the SIESTA code", June 2007 (Centre Européen of Calcul Atomique et Moléculaire, Lyon, France) 53 participants.
  (http://www.cecam.fr/index.php?content=activities/pastTutorials&action=details&wid=141)

- Lecturer in the "1st Summer School in Theoretical and Computational Chemistry of Catalonia", June 2007 (Barcelona, Spain) 40 participants.
  (http://www.xrqtc.cat/xrqtc)

- Lecturer in the "Efficient density functional calculations: hands-on tutorial on the SIESTA code", November 2007 (San Sebastián, Spain) 43 participants.

- Lecturer in the "International Workshop in Computational Materials Science", November 2008 (Cairo, Egipt).

- Lecturer in the "Introductory course of SIESTA" May 2009 (Barcelona, Spain) 48 participants.

Other

- According to the ISI Web of Knowledge (May, 17 2010):
  Total number of citations: 3408
  Average number of citations per article: 110
  Most cited paper (not first author): 2037
  Most cited paper (first author): 372
  4 papers with more than 150 citations
  8 papers with more than 50 citations
  h-factor: 17

- Extensive experience in scientific computing, including programming languages, mathematical libraries, data storage and visualization.

- Mantainer of major scientific computing codes: SIESTA, MONTEC.

- Active referee in Nature, Physical Review Letters, Physical Review B, Applied Physics Letters, Europhysics Letters, Journal of Physics D: Applied Physics, Applied Surface Science, Physica Status Solidi b, Journal of Physical Chemistry, Material Research Society Symposium Proceedings, Modelling and Simulation in Materials Science and Engineering, New Journal of Physics, Phase Transitions, Physics Letters A, Journal of Physics and Chemistry of Solids, Journal of Physics A: Mathematical and Theoretical, Journal of Theoretical and Computational Nanotechnology.

- Active referee for proposals funding agencies, such as the Department of Energy of the USA, Agence Nationale de la Recherche (France), and Fonds de la Recherche Scientific (Belgium).

- The paper published in Nature was chosen as highlight of the week.

- The paper J. Phys.: Condens. Matter **20** 064208 (2008) was chosen as one of the top papers 2008 showcase by the editorial board of the review.

- Some of my first works, done under the auspicies of Motorola INC, were used to patent the manufacturing process of the (by that time) smallest transistor in the world.

List of speakers

List of invited lecturers

- Julian D. Gale (julian@ivec.org)
  Curtin University of Technology, Perth, Australia.
- Alberto García (albertog@icmab.es)
  Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Barcelona, Spain.
- Javier Junquera (javier.junquera@unican.es)
  Universidad de Cantabria, Santander, Spain.
- Andrei Postnikov (postnikov@univ-metz.fr)
  Université Paul Verlaine, Metz, Francia.
- Daniel Sánchez-Portal (qsapod@sc.ehu.es)
  Donostia International Physics Center, DIPC-CSIC, San Sebastián, Spain.
- José Antonio Torres (jose.torres.alonso@uam.es)
  SIESTA manager, Universidad Autónoma de Madrid, Madrid, Spain.

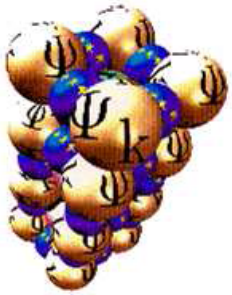
List of assistants in practical sessions

- Pablo Aguado-Puente (pablo.aguado@unican.es)
  Universidad de Cantabria, Santander, Spain.
- Marcos Verissimo-Alves (marcos.verissimo@unican.es)
  Universidad de Cantabria, Santander, Spain.
- Esteban Stafford (esteban.stafford@gestion.unican.es)
  Universidad de Cantabria, Santander, Spain.

LIST OF ATTENDEES

Name	Age	Nationality	Affiliation	Country
MIKHAIL AKHUKOV	28	Russia	RADBOUD UNIVERSITY	NETHERLANDS
VALENTIN ALBA	43	Spain	U.N.E.D.	SPAIN
LUDOVIC BRIQUET	28	Belgium	CRP GABRIEL LIPPMANN	LUXEMBOURG
PEPA CABRERA-SANFÉLIX	32	Spain	DONOSTIA INTERNATIONAL PHYSICS CENTER	SPAIN
DIEGO CARRASCAL	35	Spain	UNIVERSITY OF OVIEDO	SPAIN
ENRIQUE COMESAÑA	32	Spain	UNIVERSITY OF SANTIAGO DE COMPOSTELA	SPAIN
SERGIO CONEJEROS	29	Chile	UNIVERSITY OF BARCELONA	SPAIN
GRISELDA NOEMI GARCÍA	39	Argentina	CATHOLIC UNIVERSITY OF CHILE	CHILE
NURIA GARCÍA	24	Spain	UNIVERSITY OF BARCELONA	SPAIN
HANNES HUEBENER	29	Germany	ECOLE POLYTECHNIQUE OF PARIS	FRANCE
ELISA JIMÉNEZ	25	Spain	UNIVERSITY OF BASQUE COUNTRY	SPAIN
KAREN JOHNSTON	34	United Kingdom	MAX PLANCK INSTITUTE FOR POLYMER RESEARCH	GERMANY
SMAGUL KARAZHANOV	46	Uzbekistan	INSTITUTE FOR ENERGY TECHNOLOGY	NORWAY
JAROMIR KRYSZCZAK	27	Poland	MARIA CURIE-SKLODOWSKA UNIVERSITY	POLAND
XOCHITL LÓPEZ-LOZANO	37	Mexico	THE UNIVERSITY OF TEXAS AT SAN ANTONIO	U.S.A.
LUDOVIC MARTIN	30	France	UNIVERSITY OF BASQUE COUNTRY	SPAIN
GONZALO RECIO	23	Spain	UNIVERSITY OF MADRID	SPAIN
ÁNGELA ROJAS		Colombia	NATIONAL UNIVERSITY OF COLOMBIA	COLOMBIA
JUAN SALAFRANCA	32	Spain	UNIVERSITY OF TENNESSEE	U.S.A.
SUCHISMITA SANYAL	33	India	GENERAL ELECTRIC INDIA	INDIA
JING SHEN	29	China	CENTRALE RECHERCHE SA	FRANCE
M. BEGOÑA TORRES	41	Spain	UNIVERSITY OF BURGOS	SPAIN
MONTSERRAT VALLEJO	26	Spain	UNIVERSITY OF CANTABRIA	SPAIN
COLIN VAN DYCK	23	Belgium	UNIVERSITY OF MONS	BELGIUM

Psi-k Network : Towards Atomistic Materials Design



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PSI-K WORKSHOP FINANCE REPORT

Title of the Workshop	Efficient density-functional calculations with atomic orbitals: a hands-on tutorial on the SIESTA code
Workshop Organisers	Javier Junquera and José Antonio Torres
Location of the Workshop	Santander, Cantabria, Spain
Dates of the Workshop	June 7th- June 10th 2010
Total Grant from Psi-k	5,000 €

EXPENDITURE

WORKSHOP DELEGATES / SPEAKERS			
Name and Country of Claimant	**Travel**	**Accommodation**	**Total (€'s)**
Julian D. Gale (British citizen working in Australia)	101.66 €	240.00 €	341.66 €
Alberto García (Spain)	253.17 €	240.00 €	493.17 €
Javier Junquera (Spain)	0.00 €	0.00 €	0.00 €
Andrei Postnikov (France)	155.50 €	420.00 €	575.50 €
Daniel Sánchez-Portal (Spain)	0.00 €	240.00 €	240.00 €
José Antonio Torres (Spain)	149.34 €	420.00 €	569.34 €
Hotel expenses for 23 students (breakfast included): Check-in: Sunday, June 6th 2010 Check-out: Thrusday, June 9th 2010		5520.00 €	5520.00 €
		Total Travel & Accommodation	**7499.67 €**

WORKSHOP REFRESHMENTS / CONFERENCE DINNERS			
Date	**Tea / Coffee**	**Lunch / Dinner**	**Total (€'s)**
Coffe breaks during the whole conference (from June 7th to June 10th) for all the students and speakers	542.00 €		542.00 €
Lunchs during the whole conference (from June 7th to June 10th) for all the students and speakers		1429.59 €	1429.59 €
Welcome dinner for the invited speakers, June 6th		258.27 €	258.27 €
Farewell dinner for the invited speakers, June 9th		281.40 €	281.40 €
		Total Refreshments	**2511.26 €**

MISCELLANEOUS EXPENDITURE	
Details	**Total (€'s)**
40 Pendrives with the logo of Siesta	534.80 €
Payment to the Fundación Leonardo Torres Quevedo (who performed the administrative work in the organization of the school.	750.00 €
Total Miscellaneous	**1284.80 €**

Total Travel & Accommodation	**7499.67 €**
Total Refreshments	**2511.26 €**
Total Miscellaneous	**1284.80 €**
TOTAL EXPENDITURE	**11295.73 €**