SIESTA selected as one of the most important breakthroughs in physics

(via ICN2)

The Journal of Physics: Condensed Matter celebrates its 50th anniversary by compiling its 12 most influential articles. Among the selected breakthroughs there is the article presenting SIESTA code. SIESTA is a tool to perform electronic structure calculations and simulations of the dynamics of molecules and solids used all over the world, with Prof. Pablo Ordejón, Director of ICN2, among its authors and original creators.

On the occasion of the celebration of its 50th anniversary, the *Journal of Physics: Condensed Matter* (a prestigious European journal of solid state physics) has made a selection of the most important articles published in the journal. In this short list of papers readers will find relevant studies from acclaimed scientists, such as **J. Michael Kosterlitz** and **David J. Thouless**, both recently awarded with the Nobel Prize in Physics 2016. Many of them are seminal articles that opened a whole new research area. One of the selected breakthroughs is the SIESTA method and code. Prof. **Pablo Ordejón**, Director of ICN2 and Group Leader of the ICN2 *Theory and Simulation* Group, is among the authors of the paper presenting SIESTA in 2002. This work accumulates over 6.000 citations, becoming the eighth most cited paper over all scientific fields in the history of Spain, and the fourth around Barcelona (the first three articles have more than fifty authors, while SIESTA has only seven).

The highlighted article describes the theoretical foundations of SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms), an original method and a computer code that has recently turned into open access software. It is able to perform electronic structure calculations and molecular dynamics simulations of molecules and solids. The tool was a huge novelty back in 2002 and is widely used, hence the reason of its growing number of citations.

A distinctive feature of the program is that the simulations are run with an atomic detail of the system under study, and using only the previous knowledge of the chemical species involved, without any other

experimental input or parameters (what is called "ab-initio" or "from first principles"). Unlike most simulation software used in biology and in much of materials science, the method makes no use of previous experimental information: it only uses the basic laws of electromagnetism and quantum mechanics to be able to predict with precision the properties and behaviour of the atoms in the molecule or the solid. Using this method, more accurate predictions can be obtained, although the calculations become more complex.

SIESTA code represented a paradigm shift

The importance of the article is not only about the possibilities of SIESTA and their applicability. It also represented a paradigm shift: SIESTA works around numerical atomic orbitals, in contrast with the mainstream of the community in the nineties, which was the method of plane-waves. This change of the basis set led the computational method (DFT, Density Functional Theory) used in SIESTA into a more intuitive picture of electronic structure and opened the door to more simple calculations, requiring less computational resources, and able to study more complex materials.

A key aspect of the method is that, using a local representation of atomic orbitals, the computer effort increases linearly with the number of atoms, while other approaches scale with the cube of the number of atoms. This way, simulations of hundreds of atoms were, for the first time, possible in small workstations thanks to the code initially designed by a small team of friends and collaborators. Nowadays, much of the effort in the development of SIESTA is devoted to allow the use of the extreme power of modern supercomputers, which will reach the exascale (1018 operations per second) in the near future. Projects like the MaX Center of Excellence in "Materials Design at the Exascale", in which the group of Prof. **Pablo Ordejón** participates, are examples of this trend towards materials design and discovery through High Performance Computing.

A core team working together since 2002

SIESTA was a relevant breakthrough, and still is today. Prof. **Pablo Ordejón**, Prof. **Emilio Artacho**, Ikerbasque Research Professor and Theory Group Leader at Nanogune (San Sebastián), and Prof. **José M. Soler**, Professor at the Condensed Matter Physics Department of Autonomous University of Madrid, came up with the original idea. Anyway, SIESTA would not have become a widespread tool for advanced materials research without the contribution of other members of the core team: Prof. **Julian D. Gale**, Professor of Computational Chemistry at Curtin University (Australia), Dr **Alberto García**, Research Scientist at ICMAB-CSIC, Prof. **Javier Junquera**, Research Professor at the Earth Sciences and Condensed Matter Department of University of Cantabria, and Dr **Daniel Sánchez-Portal**, Research Scientist at the Materials Physics Center (CSIC-UPV) in San Sebastián.

The authors of the 2002 article have been working together with many other new collaborators. Special mention is deserved by Dr **José María Cela**, Director of the Computer Applications for Science and Engineering Department of Barcelona Supercomputing Center, and his Group, to maintain the SIESTA code updated and available for the international scientific community.

For those interested in working with SIESTA, ICN2 organises on November 9, 10 and 11 2016 the Module 7 of the ICN2 Open Knowledge Program, devoted to some of the advanced electronic transport simulation modules present in the SIESTA code.

Article reference

JPhys 50th anniversary: viewpoints collection

iopscience.iop.org/0953-8984/focus/JPhys50-viewpoints

José M Soler, Emilio Artacho, Julian D Gale, Alberto García, Javier Junquera, Pablo Ordejón and Daniel Sánchez-Portal. **The SIESTA method for ab initio order-N materials simulation**. Journal of Physics: Condensed Matter, 2002, Volume 14, Number 11.

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