SIESTA-PRO: Professional Software Ready for Industry

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Abstract

Simune Atomistics S.L. (SIMUNE) [1] is a company launched in 2014 as a joint venture of a group of scientific experts and the Nanoscience Cooperative Research Center CIC nanoGUNE (www.nanogune.eu). SIMUNE was created to capitalize the experience and know-how of a group of scientists, international experts in computational simulations of materials(http://www.simune.eu/index.php/about-us).

In 2015, SIMUNE established a strategic partnership with SIESTA[2]. SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) is both a method and its computer program implementation, to perform efficient electronic structure calculations and *ab-initio* molecular dynamics simulations of molecules and solids.

This workshop will cover the SIESTA package, the product SIESTA-PRO, and the support service offered by SIMUNE. SIESTA-PRO is the Commercial Software currently under development by SIMUNE on top of the existing SIESTA code to facilitate the professional use of the SIESTA code.

The main capabilities implemented on the current version of the SIESTA code, as well as the features under development will be presented.

Next, the SIMUNE protocols for the generation of pseudopotentials and the construction of basis sets of strictly localized numerical atomic orbitals will be introduced.

Finally, a detailed view of the post-processing SIESTA-PRO analysis tool will be given.

References

[1] www.simune.eu
[2] J. M. Soler, E. Artacho, J.D. Gale, A. García, J. Junquera, P. Ordejón and D. Sánchez-Portal, J. Phys.: Condens. Matter 14 (2002) 2745

Acknowledgments

SIMUNE has received funds to develop the project: SIESTA -PRO - Spanish Initiative for Electronic Simulations with Thousands of Atoms: Open Source code with professional support and warranty. The project (RTC-2016-5681-7) has been funded by the Spanish Ministry of Economy, Industry and Competitiveness and has been co-financed by the European Structural and Investment Funds with the objective to promote the technological development, innovation and quality research.

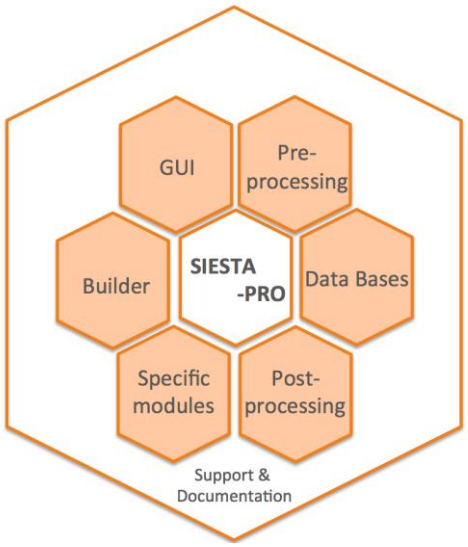

Figure 1: Schematic representation of the modules constituting SIESTA-PRO