POST-DOCTORAL RESEARCH POSITION IN THE SIMULATION AND MODELIZATION GROUP

OPTIMIZATION OF OPTICAL RESPONSE CALCULATIONS WITHIN THE SIESTA SOFTWARE PACKAGE: APPLICATIONS TO NANOPLASMONICS

Materials Physics Center (Donostia / San Sebastián)

The Modelization and Simulation Group at CFM offers a postdoctoral (1+1 years) position to work with Prof. Daniel Sánchez-Portal.

The research will focus on the improvement and optimization of the recently developed capabilities to compute the optical response of large molecules and clusters at the TDDFT level using the SIESTA code (https://departments.icmab.es/leem/siesta/). Linear response TDDFT has been implemented as a post-processing tool written in Python, called PyNAO [P. Koval, M. Barbry and D. Sánchez-Portal, Comp. Phys. Comm. 236, 188-204 (2019)]. Initial work will focus in the optimization of the algorithms, as well as cleaning and documenting the existing code. Simultaneously, the software will be applied to relevant problems on the field of nanoplasmonics and photovoltaic materials in collaboration with other theory groups at CFM (see https://cfm.ehu.es/ for more information). Additionally, we will explore the possibility to use the methodology developed within PyNAO to expand products of orbitals as a route to speed up the current implementation of the calculation of the matrix elements of the exchange interaction to use hybrid functionals within SIESTA.

The work will be performed in collaboration with Dr. P. Koval at Simune Atomistics and Prof. E. Artacho at CIC-nanoGUNE in Donostia/San Sebastián (Spain), Dr. M. Barbry in Eindhoven (Netherlands), and Dr. A. García at ICMAB-CSIC in Barcelona (Spain).

The positions will be funded by the IKUR strategy. The IKUR program has been launched by the Education Department of the Basque Government to boost Scientific Research in specific strategic areas and to position the Basque country at the forefront of international research in those fields.

The selected candidate will be hired by the Research Association MPC - Materials Physics Center. The salary will be 34.780,80€ (postdoc) before taxes for the first year. Preferred starting date should be during the first trimester of 2022.

Candidates must hold a PhD in Physics/Chemistry/Material Science/Computer Science.
The candidate should have as well:

- Experience in the development of scientific software (preferably for electronic structure or quantum chemistry calculations);
- Strong knowledge of computational methods;
- Knowledge of Python and Fortran programming language
- Experience with git and CICD way of working
- Experience with Bash scripting and Unix/Linux environment
- Past experience with Siesta and/or PySCF software are a plus

Suitable candidates can apply for this position sending by email to jobs.cfm@ehu.eus the following information before December 22 with the subject label “Postdoc CFM-Siesta”:

1- An updated Curriculum Vitae, including a list of publications. (50%)
2- A presentation letter with declaration of interests (max. 1 page). (15%)
3- Two reference letters and/or contact email of two potential referees. (35%)

General enquiries or questions about this position should be submitted by email to: jobs.cfm@ehu.eus with the subject label “Postdoc CFM-Siesta” where “Postdoc CFM-Siesta”.