5 PhD Research Fellowships in Computer Simulations, University of Aveiro, Portugal.

Five PhD positions funded by National and European programs are available to study novel materials and molecules with Density Functional Theory (DFT), wavefunction and tight-binding simulations under the supervision of Dr. Manuel Melle-Franco, at CICECO – Aveiro Institute of Materials, Portugal.

We are searching for potential **candidates with a strong interest in modeling and a good background in chemistry, physics or molecular biology** to work in technological multidisciplinary projects funded nationally and by the FET-OPEN, Pathfinder and M-ERA.NET European programs.

All projects are highly multidisciplinary with a large experimental input from several national and international collaborators. Available research topics are:

1. Fundamental studies on 2D materials with exotic electronic properties such as twisted graphene
2. biomolecules for green electronic devices such as proteins and synthetic peptides
3. helping develop and refine nanomaterials for new cancer treatments.
4. Modelling novel porous framework materials for:
    a. electronic devices
    b. new batteries
    c. detecting pharmaceutical pollutants

The chosen candidates will join Manuel Melle's computational group currently integrating 1 bachelor student, 1 M.Sc. student, 3 PhD students, 1 Postdoc, 2 auxiliary researchers and 1 principal researcher. The group uses several state of the art workstations and has access to a cluster with nearly 1.5k cores, national and international HPC facilities and several simulation software licenses. The group focuses on understanding and predicting computationally the properties of novel molecules and materials and produces a sizable high-visibility research output (updated list of publications). Linux/Unix administration and programming experience is not mandatory but will be considered an asset.

Eligibility: Master degree or equivalent in Chemistry, Physics, Physics Engineering, Materials Science, Biochemistry or related. Note that the degree must be, according to current legislation, legally recognized in Portugal at the start of the fellowship. This can be easily obtained from degrees in countries with automatic degree and diploma recognition in Portugal.

For more details on conditions, eligibility and how to apply, formal and informal inquiries may be directed to Dr. Manuel Melle-Franco (manuelmelle.group@gmail.com**).**

Funding

1. Alternative SuperConducting Superlattice (SuperSuper). European Union, M-ERA.NET Program.
2. Fabricating and Implementing Exotic Materials from Covalent Organic Frameworks (FantastiCOF). European Union, Pathfinder program (ref.101046231).
3. Engineered Conductive Proteins for Bioelectronics (EPROT), European Union, Future and Emerging Technologies FET-Open program (ref: 964593).
4. Multifunctional carbon nanocapsules for highly efficient neutron cancer therapy, (C@RBONCT), Foundation for Science and Technology, FCT.
5. Redox-active Metal-Organic Frameworks as Electrode Materials for Lithium-Ion Batteries (RedoxMOFs). Foundation for Science and Technology, FCT (ref: PTDC/QUI-ELT/2593/2021).
6. Supported Covalent Organic Frameworks for the Monitoring of Pharmaceutical Pollutants (CHARM). National, Foundation for Science and Technology, FCT (PTDC/QUI-OUT/2095/2021).
7. Graphene for a New Generation of Electronics (GRAPH-ELE). National, Foundation for Science and Technology, FCT (IF/00894/2015).

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