CNR-IOM Cagliari

Post-Doc in Computational Physics

Physics-based and Machine Learning Force-Fields for Hybrid Perovskites

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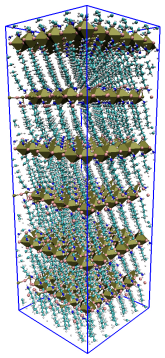
Post-doc position on "*Physics-based and Machine Learning Force-Fields for Hybrid Perovskites*" available at CNR-IOM Cagliari in Mattoni group **(https://www.dsf.unica.it/~mattoni) .**

Contract and Salary

The two-year position will start in March/April 2024. Net salary per month ranges between 1600 and 2200 euros depending on the candidate research experience.

Activity and Projects



The successful candidate will play a significant role in developing and applying molecular dynamics methods to the study of **crystal growth** and **stability** of non-toxic 2D/3D **hybrid perovskites**.

The candidate will develop **physics-based force-fields** (of the MYP family by Mattoni et al.) as well as **machine-learning models** (based on atomic cluster expansion) for novel perovskites. Atomistic datasets and trajectories will rely on **ab initio calculations**.

The computational activity will be developed within ongoing **collaborative projects** involving several international experimental and theoretical groups (University of Cagliari, Kyoto University, Cambridge University, University of Groningen).

Criteria

Eligible candidates should have a **PhD** degree in physics or chemistry or materials science or related disciplines and a strong motivation in theory and computational methods for condensed matter physics.

The candidate should demonstrate experience with **atomistic methods** such as DFT calculations (e.g. Quantum Espresso, VASP, etc) and/or classical molecular dynamics (e.g. LAMMPS, DL_POLY).

Previous knowledge of UNIX/Linux environment and **programming** (either Fortran2008 and/or C/C++ and/or Python) is necessary. Experience in machine learning methods is preferred but not mandatory.

Very good communication skills in **English** and marked **enthusiasm** for research.

Host Institution and Location

CNR-IOM Cagliari is part of the Istituto Officina dei Materiali (www.iom.cnr.it) and it is located at the Physics Department of the University of Cagliari.

Cagliari is the main metropolitan area of the Sardinia island (renowned for beautiful beaches) with an above-average quality of life (https://expiter.com/province/cagliari/) and good airplane connections.

Application

Informal enquiring and a **CV** should be sent as soon as possible by **email** to: Alessandro Mattoni (CNR-IOM Cagliari, mattoni@iom.cnr.it)