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|  |  | Post-Doc in Computational Physics  ***Physics-based and Machine Learning Force-Fields for Hybrid Perovskites***  Tel.: +39 070 6754875 Fax: +39 070 6754892  EMAIL: [mattoni@iom.cnr.it](mailto:mattoni@iom.cnr.it) |
|  |  | Post-doc position on “*Physics-based and Machine Learning Force-Fields for Hybrid Perovskites”* available at CNR-IOM Cagliari in Mattoni group **(**[**www.dsf.unica.it/~mattoni**](http://www.dsf.unica.it/~mattoni) **) .** |
| Contract and Salary |  | The two-year position will start in March/April 2024. Net salary is within 1600 to 2200 euros net per month depending on the candidate research experience. |
| Activity |  | 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 developed by Mattoni et al.) as well as **machine-learning models** (based on atomic cluster expansion) for novel perovskites. **Ab initio calculations** will be necessary to generate atomistic datasets and trajectories.  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). |
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| Criteria |  | Eligible candidates should have a Ph.D. degree in physics or chemistry or materials science 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. by 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 Locaiton |  | CNR-IOM Cagliari is part of the Istituto Officina dei Materiali ([www.iom.cnr.it](http://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 to: Alessandro Mattoni (CNR-IOM Cagliari, [mattoni@iom.cnr.it](mailto:mattoni@iom.cnr.it)) |