

# Two Research Post-Doctoral Positions open at the University of Modena and Reggio Emilia on atomistic modelling of battery materials

The High-Performance Computing for Material Design group at the Department of Physics, Informatics and Mathematics (FIM) ([www.fim.unimore.it](http://www.fim.unimore.it)) has an opening for two Research positions in the area of atomistic modelling of interfacial phenomena in Li ion batteries. The initial appointments are for one year but they can be extended upon mutual agreement and satisfactory research performance for a second year. Salary will be commensurate with experience, training and qualifications: the amount of the monthly net salary will be in the range 1400.00 – 2000.00 euro.

The projects:

1. Study of eco-friendly polymeric binders for electrodes of Lithium Ion batteries by atomistic simulations
2. Atomistic Simulations of the Electrode-Binder Interfaces

involve the use of material modelling (ab-initio simulations, and classical and ab-initio molecular dynamics) to simulate the properties of polymeric eco-friendly self-healing binders and their interaction with the active material surfaces to be compared with the results of the experimental groups actively collaborating in the projects.

The positions are funded by MUR (Italian Ministry of University and Research) under the PRIN 2022 Project “BIONIC - Binders with high iONic Conductivity for fully sustainable Li-ion cells”.

Successful candidates will hold a PhD degree in a relevant discipline (Computational Physics, Chemistry, Physics, Material Science or similar) and will have demonstrated expertise in two or more of the following areas: Density Functional Theory, Ab initio Molecular Dynamics, Classical Molecular Dynamics, Advanced Sampling methods, and optimization methods. Programming and analytical skills, and knowledge of high performance computing are desirable.

The deadline for applying is 16<sup>th</sup> November 2023, 1 p.m. (CET)

Interested candidates should send their (a) CV containing a list of publications, (b) a cover letter describing their background, key research accomplishments, and capability in modelling material systems, and (c) names, email, and telephone numbers of two references by email to Prof. Rita Magri ([rita.magri@unimore.it](mailto:rita.magri@unimore.it)).