PhD position available - University of Limoges - CNRS: Development of machine learning interatomic potentials for complex oxide-based cathodes.

A Ph.D opening is available at the Institute of Research on Ceramics (IRCER), University of Limoges, CNRS UMR 7315 (France)

PhD context and project:
The current PhD proposal is a part of a collaborative project entitled "Advanced Modelling as a Strategy to design glass and glass-ceramic materials for Energy Storage applications (AMSES)" funded by the French National Research Agency ANR.
This project focuses on the study of complex oxide cathode materials for Alkali ion batteries. In particular, AMSES focuses on Sodium glasses (G) and glass-ceramic (GC) materials as they can achieve safety, environmental sustainability, and simplified design. Yet, the lack of understanding of both their structures and the mechanisms underlying ion dynamics prevents practical applications. In AMSES we combine DFT, first-principles molecular dynamics, machine leaning techniques and laboratory synthesis and characterization to achieve a rational design and elaboration of novel G and GC materials.

Within AMSES, we will exploit data-bases issued from DFT/FPMD calculations in order to develop versatile machine learning interatomic potentials for the class of the considered materials. Approaches such as Gaussian Approximation Potential, Deep Potential Molecular Dynamics, and High-Dimensional Neural Network Potentials will be considered. The obtained machine learning potentials will be used to refine glass compositions and to perform large-size and long-lasting simulations of the targeted G and GC materials and interfaces.

The selected candidate will work closely with the team of Dr. Carlo Massobrio (DFT/FPMD aspects) at the Institute of Physics and Chemistry of Materials of Strasbourg (IPCMS) with possible stays at IPCMS, and with Prof. Gaëlle Delaizir (synthesis and characterization) at IRCER.

Qualifications:
Qualified candidates are required to hold a Master degree in physics, chemistry, material science or condensed matter theory with an excellent academic track record and proficiency in Python programming. Knowledge of other programming languages (Fortran, C and/or C++) is a plus.
A minimal background knowledge of machine learning, density functional theory and/or classical molecular dynamics techniques is highly advantageous.

How to apply:
The interested PhD candidate should send a single PDF file containing: curriculum vitae, publication list (if any), and the list of passed examinations and relative marks. In addition, the interested PhD candidate should also express his/her motivation in a cover letter and arrange confidential letters of recommendation to be sent to the contact points below. Only complete applications will be processed.

Assessment:
Acceptance of candidates is subordinated to a further selection from the Doctoral School of the University of Limoges. A mandatory oral presentation will be scheduled for the selected candidates who will be notified of acceptance.

Appointment:
The PhD project is expected to start on October 2021 and the position is intended for three years.
Application Deadline: May 7, 2021.

Further information available at: https://www.ircer.fr/

Contact Information Points:

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