

Ph.D position: data-driven materials modelling a ... (No replies)



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in_cadars
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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 PhD proposal is integrated in a Common Research Lab between the French Commissariat à l'Énergie Atomique (CEA) and the IRCER (CNRS, University of Limoges).

In a context where data-driven science undergoes rapid developments in most fields of research, innovative numerical tools and platforms have been developed around the world to generate, store and retrieve materials structures and properties in rapidly-growing databases of theoretical materials. In combination with databases of experimental materials, such theoretical databases offer opportunities to search for new families of structures targeting certain physical properties to outperform existing materials in a wide range of technological applications.

The performance of electromagnetic and electronic devices, for example, is often limited by the absence of dielectric materials satisfying constraints on both their preparation process (stability, compatibility with a silicon support) and their dielectric constant. We propose to develop a largely-automatized strategy to systematically predict this particular property as a function of chemical composition and atomic structure of materials satisfying the energetic and structural criteria compatible with their usage in the targeted applications, notably as "high-k" dielectric materials.

The PhD project will involve modeling at the density functional level of theory of static (electronic contribution) and dynamic (ionic contribution) dielectric permittivity, structure prediction, as well as systematic screening of potentially-stable crystalline oxide compositions in a large panel of existing experimental and theoretical databases. A large part of the project will be dedicated to the automatization of these protocols by exploiting existing libraries and platforms dedicated to high-throughput materials modelling. With the automatization in place, it will gradually become possible to train deep learning algorithms to both predict dielectric properties to a level of precision comparable to DFT modeling and simultaneously identify compositions and crystalline structures satisfying the experimental constraints of processes.

The selected candidate will work within a renowned ceramics laboratory with numerous connections with advanced technologies industries focusing on materials processes and applications, as well as a strong expertise in fundamental materials synthesis, characterization and modelling. The modelling team has regular access to local and national high-performance computing centers with expertise on code development, optimization, scaling and offering various training opportunities.

Qualifications:

Qualified candidates are required to hold a Master degree in quantum chemistry, physics, 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 density functional theory, classical molecular dynamics techniques, machine learning, and/or high-throughput modelling would be highly valuable.

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 motivations in a cover letter (1 page maximum) 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 2022 and the position is intended for three years.
Application Deadline: May 31, 2022.

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

Contact Information Point:

Dr. Sylvian Cadars
e-mail: sylvian.cadars@unilim.fr

Dr. Assil Bouzid
e-mail: assil.bouzid@unilim.fr

Institute of research on ceramics ([IRCER](#))
European Center of Ceramics
12 Rue Atlantis, 87068 Limoges (France)