Ph.D Position
"Ab-initio Design of High Entropy Materials"

A Ph.D position on the exciting topic of "Ab-initio design of high entropy materials" is available from January 2024 (non-negotiable) at the Atomic-scale Modelling and Crystal Chemistry group, Institute of Research for Ceramics Laboratory (CNRS), University of Limoges. The work will be carried out under the joint supervision of Dr. Santanu Saha (Junior Professor), Dr. Assil Bouzid (CNRS Researcher) and Dr. Samuel Bernard (CNRS Researcher) at the IRCER Laboratory, Limoges (France).

The Ph.D project will provide an exciting opportunity for the suitable candidate to learn and gain hands on experience on different state of the art computational material design paradigms - density functional theory, high throughput screening, machine learning along with the exciting topic of high entropy materials. The candidate will also greatly benefit from the expertise of the in-house and collaborating national and international experimental teams.

The application deadline is on 15 September, 2023. (Details provided below)

Keywords: high entropy materials, density functional theory, computational material design, workflows, machine learning

Thesis Project

High entropy materials in general refer to the class of compounds constituting five or more elements giving rise to unusual properties. These properties are of interest in different application areas such as electronics, green energy, etc. [1,2].

Given a crystal lattice with well defined atomic sites, the multitude of possibility of decorating these sites with different elements from the periodic table is astronomically large. This vast phase space (atomic arrangement) and chemical space (choice of elements) thus gives rise to high entropy. Typically chemically similar elements with equi-molar composition are chosen for mixing in a high entropy material. Amongst all these possibilities only a small percentage is stable, due to myriad of reasons such as inherent elemental and material chemistry, disorder, thermodynamics, cocktail effects, etc. This makes the identification and experimental realisation of potential compounds challenging.

One of the primary objective of the Ph.D project will be the development of simulation workflows based on different material design paradigms (crystal structure prediction, high-throughput screening, machine learning, etc.) to accelerate the search of different classes of high entropy materials and (ii) apply the developed workflow to a specific family of high entropy material. The identified potential compositions will be investigated throughly via first-principles based approaches.

Interested candidates can contact either of the personnels for an informal enquiry :
Dr. Santanu Saha : highentropy.materials@gmail.com
Dr. Assil Bouzid : assil.bouzid@unilim.fr

[1] "High Entropy Alloys : A Critical Review", M.H. Tsai et. al., Mater. Res. Lett. 2, 107-123 (2014)
[2] "High Entropy Ceramics", C. Oses et. al, Nat. Rev. Mater. 5, 295-309 (2020)

Candidate Profile

We seek a motivated master student from subject areas of Physics, Chemistry, Material Science, Chemical Engineering or other streams with relevant courses in Condensed Matter, Quantum Mechanics, Thermodynamics, Statistical Physics and Computational Programming. The candidate is expected to have good hands on programming experience along with understanding of condensed matter physics. The list of skill set we are looking for in an ideal candidate is as follows : -

Essential

(i) Good foundation in regular Bachelor/Master courses along with condensed matter, quantum mechanics, thermodynamics, statistical physics.
(ii) Experience of programming in Python and/or Fortran/C/C++
(iii) Good writing and communication skills in English
(iv) Self motivated, independent and team player
(v) An interest in programming, computational material design, big data, data analysis, machine learning, material science, interdisciplinary topics

Desirable

(i) Acquaintance with density functional theory or other first-principles formalisms and calculations with different ab-initio packages
(ii) Experience with simulation of materials and their properties
(iii) Experience in running material simulation in computing clusters, supercomputers etc.
(iv) Experience in working with machine learning tools in the context of materials based problems

How to apply

The interested candidates are requested to apply with the following list of documents to Dr. Santanu Saha (highentropy.materials@gmail.com) : -

(i) a CV
(ii) scanned copies of Bachelor and Master final mark-sheet in English/French
(iii) a short motivation letter describing their interest in the position, description of the master's thesis (project goal and contribution) and experience in computational programming and simulation (if any) within 2 pages (A4)
(iv) List of preprint/publication(s) if any with mention of their contribution
(v) Contact of at-least two to a maximum of three references

The candidates will be asked explicitly to organise for the references via mail during the final stages of selection. One of the referees should be your thesis/project supervisor.

Application Details

Starting Date : January 2024 (non-negotiable)
Duration : 3 years
Salary : €2100 / month (gross) subject to increase based on the latest French regulation
Institute : Axis 3 - Multiscale Structural Organisation of Materials
Institute of Research for Ceramics Laboratory (CNRS), University of Limoges
Limoges 87068, France

Please send the application with all the relevant documents in a single pdf file to Dr. Santanu Saha with subject "PhD HEMAT Jan2024" at highentropy.materials@gmail.com

Application Deadline : 15 September, 2023