Ph.D Position
“First-Principles Exploration of High Entropy Materials”

One fully funded Ph.D position is available on the exciting topic of “First-Principles Exploration of High Entropy Materials” from September 2024 at Institute of Research for Ceramics Laboratory (IRCER-CNRS), University of Limoges. The work will be carried out under the joint supervision of Dr. Santanu Saha (Asst. Professor), Dr. Assil Bouzid (CNRS Researcher) and Dr. Samuel Bernard (CNRS Researcher) at the IRCER Laboratory, Limoges (France).

Application Deadline : 15 April, 2024. (Details provided below)

Thesis Project

High entropy materials refer to condensed matter systems constituing diverse chemical species (N > 5) . The intrinstic high entropy along with indivudual chemical nature of elements in these systems, has made their experimental realization feasible with unusual properties useful for different application areas such as electronics, green energy, etc. [1,2]. Thereby giving rise to new class of materials,.

The inherent vast phase space (atomic arrangement) and chemical space(choice of elements) of these high entropy materials are both interesting and challenging to address both experimentally and theoretically, particularly for structure-property relationships. Till date, physical factors such as inherent elemental and material chemistry, disorder, thermodynamics, cocktail effects, etc. has been identified as crucial factors for stabilization, as elucidated by the recent studies. Despite signifiacnt progress in experimental studies, theoretical studies are still limited considering the modelling challenges.

One of the primary goal of the Ph.D project will be the addressing these systems via first principles methodologies via simulation workflows pipeline based on high-throughput, crystal structure prediction, machine learning to (a) understand the underlying processes and (b) applying the gained know-how to accelerate the searches over other chemical systems. The identified potential compositions will be investigated throughly. There will be opportunity for experimental collaboarations.

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

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

Candidate Profile

We seek a motivated master student from subject areas of Physics, Chemistry, Material Science, Chemical Engineering or other streams with relevant background 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 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 : September 2024 (non-negotiable)
Duration : 3 years
Salary : €2100 / month (gross)
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 Sep2024" at highentropy.materials@gmail.com

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