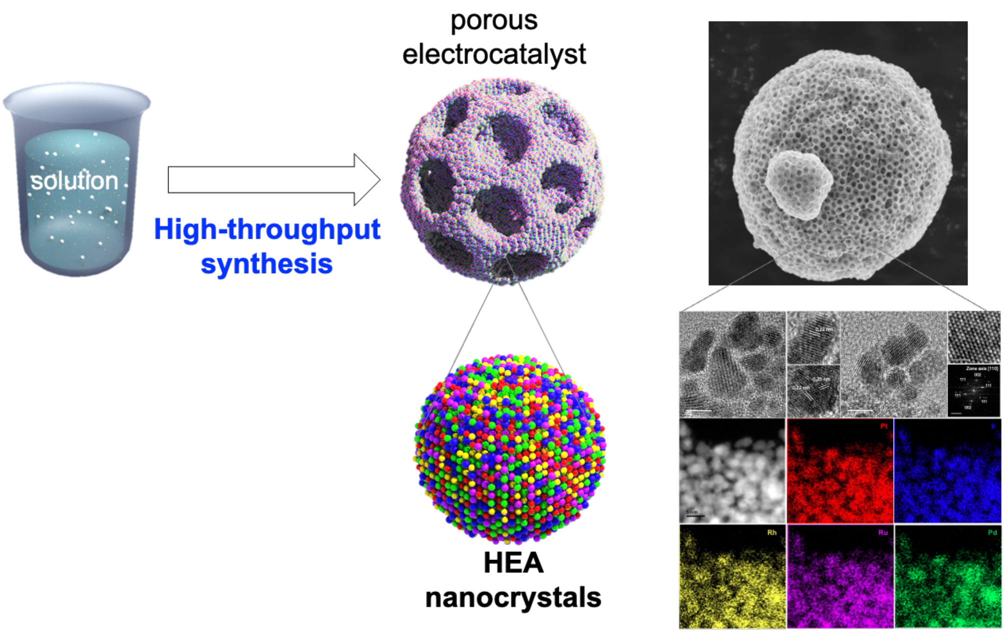
PEPR DIADEM Project

20-24 months Post-doc Position

High-throughput synthesis of porous electrocatalysts based on High Entropy Alloy nanocrystals



Why High Entropy Alloys? Originally conceptualized in the mid-2000s, high-entropy alloys (HEAs) consist of multi-metallic compounds with five or more elements, each between 5% and 35% atomic concentration. Their tunable mechanical properties quickly gained scientific interest. More recently, HEAs have been explored for **energy and catalysis applications** due to their tailored structure and composition, which affects the electronic properties of their surface sites and allows for replacing noble metals with cheaper transition metals. Research over the past years has focused on developing efficient synthesis methods for HEA nanocatalysts and testing them in reactions like oxygen and CO_2 reduction. (1) These studies find HEAs more active and stable than traditional catalysts, but controlling their properties is challenging due to the huge variety of potential chemical configurations and the difficulty of characterizing reactions that occur over very short time scales. Consequently, **selecting specific HEA configurations for targeted catalytic properties remains a complex and costly task**.

Our approach To tackle this challenge, several partners with complementary expertise teamed up to shape the **large M2P2_HEA project**. The primary objective of project is to create a multi-scale analysis methodology for high entropy alloys (HEAs) to accelerate the discovery of new electro-catalysts. This approach aims to elucidate the structure, thermodynamic characteristics and reactivity of HEAs, by combining artificial intelligence, multi-scale simulation and modeling, high-throughput synthesis, in-situ characterization and electrochemistry**.** Ultimately, this will enable the prediction of optimal composition and structure for specific catalytic applications.

What is our goal? The objective of this postdoctoral project is to develop a **high-throughput process for synthesizing macroporous materials composed of HEA nanocrystals**. The electrocatalysts will be prepared using sol-gel processing applied to metals, an approach recently introduced at Sorbonne Université to fabricate porous noble metals-based HEAs (2) as shown in the Figure.
The candidate will (i) further implement our existing process based on spray -drying (2) and (ii) develop an **innovative automated process** enabling **rapid production of a large array of different multimetallic materials**, with independent variations in metal composition and atomic percentage. The final goal is to provide a large number of samples with adjustable chemical properties to other partners for electrochemical testing, in situ microscopy, X-ray absorption, and to support machine-learning-based approaches.
This work will be conducted in the framework of the M2P2_HEA PEPR project that will involve close collaboration with several partners (Univ. Strasbourg, Univ. Paris Cité, Synchrotron Soleil, IFP Energies Nouvelles).

Profile: We are seeking a candidate with a chemistry/engineering background and experience in processing nanomaterials, porous materials, and/or catalysts, along with expertise in materials characterization techniques. A solid background in building experimental setups (and coding) is essential. Considering the collaborative nature of the project, the ideal candidate should also possess strong team-working abilities and excellent communication and writing skills.

Location/supervision: The contract duration (20-24 months) and salary will be based on the individual's profile, career stage, and prior experiences. The candidate will work at Laboratoire Chimie de la Matière Condensée de Paris at Sorbonne Université downtown Paris. The post-doc project will be supervised by Pr. Marco Faustini.

How to apply? The applicant will attach a CV including a list of publications, a short (***max*** 2 pages) research summary, and the contact of 2 references he/she worked with.

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[1] Y. Xin, S. Li, Y. Qian, W. Zhu, H. Yuan, P. Jiang, R. Guo, L. Wang, ***ACS Catal.*** **10**, 11280−11306 (2020).
[2] M. L. De Marco, W. Baaziz, S. Sharna, F. Devred, C. Poleunis, A. Chevillot-Biraud, S. Nowak, R. Haddad, M. Odziomek, C. Boissiere, D. P. Debecker, O. Ersen, J. Peron, M. Faustini, ***ACS Nano*****, 16,** 15837-15849 (2022)