IPVF 18, bd Thomas Gobert 91120 Palaiseau, France

cea isas Saclay, 91191 Gif sur Yvette, France

MISSION TITLE

PhD offer (IPVF, Palaiseau/CEA, Gif-sur-Yvette)

Innovative coatings for High-Temperature water Electrolyzers for H_2 production by Atomic Layer Deposition and DLI-CVD

POSITION DESCRIPTION

Function	Doctoral Researcher	**Contract type**	CDD
Education	Ms in Material Science, Physics, or other relevant fields	**Duration**	36 months
Working Place	Palaiseau (IPVF), Gif-sur-Yvette (CEA), Paris area	**Starting date**	From 2023, Oct 1st

IPVF IN BRIEF

IPVF - Institut Photovoltaïque d'Île-de-France, is a global Research, Innovation and Education center, which mission is to **accelerate energy transition through science & technology**. Gathering industrial PV leaders (EDF, TotalEnergies, Air Liquide, Horiba and Riber) and world-renowned academic research organizations (CNRS, Ecole Polytechnique), multi-disciplinary and international IPVF teams conduct research for clean energy technologies. Supported by the French State, IPVF is labelled Institute for Energy Transition (ITE).

IPVF at a glance: an ambitious Scientific and Technological Program (6 programs divided in 24 work packages): from tandem solar cell technologies to economy & market assessment, state-of-the art characterization, photocatalysis and breakthrough concepts; a state-of-the-art technological platform (8,000m²): more than 100 cutting-edge equipment's worth €30M, located in cleanrooms (advanced characterization, materials deposition, prototypes for fabrication, modelling…); a high-standard Education program (M.S. and PhD students). Website: https://www.ipvf.fr

CEA ISAS IN BRIEF

CEA - The French Alternative Energies and Atomic Energy Commission (CEA) is a key player in research, development and innovation in four main areas defense and security, low carbon energies (nuclear and renewable energies), technological research for industry and fundamental research in the physical sciences and life sciences. The CEA is the only French research organization to be listed in the Clarivate 2020 ranking and is the leading French research organization filing patents in Europe, according to the European Patent Office (EPO) 2021 ranking. To meet both the current and future stakes of the energy transition which is indispensable to fight climate change, the CEA has been leading research on low-carbon power systems combining nuclear and renewable energies. This research covers low-carbon power production methods, the systems used for energy storage, control and conversion, and resource management within a circular economy strategy. This wealth of expertise serves the interests of the French public authorities and industry players.

CEA at a glance, this is 21 148 employees established in nine centers spread throughout France, 37 joint research units, 710 priority patents files in 2019, 228 start-ups since 1972 and 5,6 billion euros budget. Website : https://www.cea.fr/

JOB CONTEXT

This thesis is part of a national project named ATHERM_COAT which main long-term objective is to generically demonstrate the ability to accelerate the discovery of new high performance coatings for energy transition, minimizing critical and/or toxic elements using thermodynamics and artificial intelligence.

The application and methodological demonstration case chosen here is the development of high temperature oxidation resistant coatings for Solid Oxide Electolyser Cell (SOEC) for production hydrogen, by DLI-CVD (Direct Liquid Injection Chemical Vapor Deposition) and ALD (Atomic Layer Deposition) technologies. Indeed, as part of the development of "green" hydrogen production, SOEC is currently being developed in France at the CEA and in many other countries such as Japan, the USA, Sweden and Germany. This electrolyser offers superior performance than others thanks to its high

temperature (700 - 800°C) operation, but suffers from material degradation and reduced long-term performance. To improve its performance, several types of coatings have been investigated over the last twenty years, the best ones being based on cobalt-rich spinels that can be doped with several elements (Mn, Cu, Ce, …). However, the exact nature of these coatings and its process of synthesis still need to be optimized according to several criteria (conductivity, oxidation resistance, thermal expansion coefficient, degree of criticity of the used elements, toxicity, energy cost of the coating procedure …). **The aim of this project is, in that context, to develop innovative coatings, directly deposited on the metal interconnector by DLI-CVD and ALD.**

The PhD project will integrate all the steps from the selection and testing of the precursors necessary for its synthesis, the elaboration of this coating by DLI-CVD and ALD technologies and finally the characterization of its performance in SOEC running conditions. The thermodynamic approach for the choice of precursors and the selection of the coating material will be integrated to accelerate the development of these coatings. It is a shared workload between the IPVF and the CEA, and will also benefit from the experimental platform developed by other partners in the ATHERM_COAT project. Thanks to its strong expertise on ALD, UMR-IPVF will cover several aspects of the coating deposition by ALD: molecular precursor selection, ALD deposition and characterization of thin films, growth mechanism study, in-situ instrumentation. Coating synthesis by DLI-CVD will be carried out on a DLI-CVD industrial pilot at CEA, as well as the performance tests for SOEC application. Synthesis of "optimized" coatings by combined ALD and DLI-CVD could be initiated.

MAIN MISSIONS

The doctoral researcher will benefit from IPVF and CEA expertise and unique capabilities in coating development by ALD and DLI-CVD.

She/he will integrate two dynamic and talented teams driven by innovation and results. Using their unique capabilities, her/his main missions will consist in the development of efficient coatings for SOEC for H_2 production by ALD and DLI-CVD. In particular, for ALD, the main steps will be:

- Identification of the most promising set of precursors and detailed study of their reactivity in ALD conditions,
- Development of ALD process for the preparation of inorganic thin films and growth mechanism study
- Characterization of the material typical properties relevant to the material target functionality, i.e. morphological (XRR, SEM), structural (GIXRD and Raman), composition (EDS, XPS)
- Study of the effect of annealing under different conditions (air, N_2, H_2/N_2, H_2/H_2O, ... up to 900 °C)

When relevant, the same steps using DLI-CVD (Direct Liquid Injection-Chemical Vapor Deposition) will be performed.

SOUGHT PROFILE

Knowledge	Know-how	Self-management skills
▪ Materials science ▪ Optical instrumentation ▪ Thin film characterization ▪ Inorganic chemistry	▪ Hands-on experience with thin films would be a plus ▪ Data treatment ▪ Communication of results	▪ Curious and enterprising ▪ Autonomous ▪ Organizational and collaborative skills ▪ Results-oriented

CONTACT

Cover letter, academic records and CV (including the name and contact details of at least two references) to be sent to: n.schneider@cnrs.fr and fabien.rouillard@cea.fr