Post-doctoral position available	
Job title	Post-doctoral fellowship in computational materials science https://euraxess.ec.europa.eu/jobs/687817
General information	Workplace: GREMI (Orléans, France) Contract period: 12 months Starting date: January 2021 Candidate must submit a Curriculum Vitae, a motivation letter, a copy of the PhD diploma including jury report, a copy of ID card or passport and 2 reference letters. Applications must be sent by e-mail to Dr Pascal Brault pascal.brault@univ-orleans.fr
Missions	The postdoctoral researcher will be part of the ANR project InnOxiCat dedicated to designing non-PGM catalysts for fuel cells. She/He will conduct suitable molecular simulations using advanced computing resources.
Activities	The main objective of the multi-disciplinary InnOxiCat project concerns the development of non- Pt group metal catalysts for the implementation of the next generation of hydrogen Fuel Cell (Proton Exchange Membrane Fuel Cell architecture). In this context, the InnOxiCat project makes the choice of developing titanium and zirconium oxide and oxynitride-based catalysts for the oxygen reduction reaction (ORR). To reach the InnOxiCat objectives, it is planned to design and conduct molecular simulation of synthesis of oxide and oxynitride nanoparticles (NPs) and porous thin films (PTF) as well as studying the ORR on these designed catalysts. More precisely, the molecular dynamics approach will allow predicting the morphology, the size, the composition and the structure of the catalysts. The variable charge reactive reaxFF and COMB3 force fields will be used and improved both for TiO_xN_y and ZrO_xN_y NPs and PTF growth. After completing the virtual design of the catalytic phases, Density Functional Theory (DFT) approach will allow characterizing properties such as OH adsorption which is a marker of the catalyst efficiency. Indeed, a precise study of OH adsorption on the various site of the nanocatalysts will be carried out for determining their low binding site using various DFT schemes. Simulated results will be compared to physical, chemical analysis of the materials and electrochemical tests performed in the consortium. Suggested readings: P. Brault et al, Front. Chem. Sci. Eng. 13 (2019) 324 DOI: 10.1007/s11705-019-1792-5 P.C. Jennings et al, Phys.Chem.Chem.Phys., 18 (2016) 24737 DOI: 10.1039/c6cp04194a Y Okamoto, Appl. Surf Sci. 255 (2008) 3434 DOI: 10.1016/j.apsusc.2008.09.061 G. Wang et al, Solid State Ionics 317 (2018) 15 DOI: 10.1016/j.ssi.2017.12.036 A. Seifitokaldania et al, Electrochimica Acta 141 (2014) 25 DOI: 10.1016/j.electacta.2014.07.027
Skills	The candidate should hold a PhD in the field of computational material science with emphasis on chemical and surface reactivity. Extensive practice of reactive molecular dynamics and skills on DFT and DFT coupled to MD are required. Published articles as main author are expected. • Additional knowledge on plasma synthesis of nanostructured oxide materials will be appreciated. • Fluent English both written and spoken is mandatory. Fluent French speaking is advised. • Ease to write articles, reports and presenting results at conferences and during project reviews is expected.
Context of the work	GREMI (CNRS, Université d'Orléans) has a long expertise, both experimental and with molecular simulations, in plasma processes especially in magnetron sputtering deposition of metallic and metal oxide thin films, nanoparticles, either pure or alloyed and core-shell clusters for application in catalytic H2 production, catalytic combustion, fuel cells and mechanics. ANR InnOxiCat gathers French research teams on all aspects of fuel cell design and testing. Computational resources are available at GREMI and at CASCIMODOT computing center. The AMS suite from SCM company will be available for DFT/DFT-MD simulations.
Supplementary information	The closing date for receiving applications is October 30th. The selection procedure is in 2steps: First, selecting a short list of best candidates and second, the final selection after an hearing.