PhD Proposal 2017

School: CentraleSupelec	
Laboratory: SPMS	**Web site: www.spms.ecp.fr**
Team: Functional Materials for Energy	**Head of the team: G. Baldinozzi**
Supervisor: G. Dezanneau	**Email: Guilhem.dezanneau@ecp.fr**
Collaboration with other partner during this PhD: **In France:**	 **In China:** **F. Ciucci, Hong-Kong University of Science and Technology**

Title: Modelling of oxide ion conductors for Solid Oxide Fuel Cells by molecular dynamics
Scientific field: Solid state chemistry, computational science
Key words: SOFC, Ion conductors, Molecular dynamics, Diffusion,

Details for the subject:

Title: **Molecular Dynamics simulations applied to ion conductors for fuel cells.**

Field/applications:

Materials for fuel cells, modelling, Ab initio, molecular dynamics

Context and objective:

Solid Oxide Fuel or electrolysis cells are expected to play an important role in a near future, in the field of energy. While many oxide compositions have been found experimentally for electrode or electrolyte applications, the explanation of their good performance is scarce showing the limitations of the empirical approach. By the use of molecular dynamics, we have shown that we could get highly relevant information for understanding the oxygen ion diffusion mechanisms in a series of oxides. We have also shown that we were able to provide routes for the design of new materials making the molecular dynamics method highly powerful. **The objective of the present PhD thesis is to apply Molecular Dynamics method to ion conductors used as cathodes/anodes materials in Solid Oxide Fuel Cells.**

Work:

The student, after the choice of several compositions, will realize DFT calculations in order to obtain fine parameters for the semi-empirical potentials. MD calculations will be launched so as to obtain a long range diffusion coefficients and atomic scale jump mechanism. The student will also develop tools for a statistical fine analysis of oxygen atoms jumps. The study will be realized in collaboration with our partner in Hong-Kong University of Science and Technology (Prof. F. Ciucci).

Skills:

Physics, Physical chemistry, numerical methods. Interest in simulations aspects.
Research Master. Excellence required.

Laboratory: **Lab. Structures, Propriétés et Modélisation des Solides, CentraleSupélec**
Supervisors : guilhem.dezanneau@ecp.fr ; Francesco.ciucci@ust.hk

References:

The effect of A-site and B-site substitution on $BaFeO_{3-\delta}$: An investigation as a cathode material for intermediate-temperature solid oxide fuel cells
J. Wang, M. Saccoccio, D. Chen, Y. Gao, C. Chen, **F. Ciucci**
Journal of Power Sources 297, 511–518, **2015**

Influence of isotropic and biaxial strain on proton conduction in Y-doped BaZrO3: a reactive molecular dynamics study

A. Ottochian, **G. Dezanneau**, C. Gilles, C. Knight, P. Raiteri. J.D. Gale

Journal of Materials Chemistry A, 2, 3127, **2014**

Unraveling the effect of La A-site substitution on oxygen ion diffusion and oxygen catalysis in perovskite $BaFeO_3$ by data-mining molecular dynamics and density functional theory

C. Chen, Z. Medina Baiyee, **F. Ciucci**,

Physical Chemistry Chemical Physics, August **2015**

How dopant size influences the protonic energy landscape in $BaSn_{1-x}M_xO_{3-x/2}$ (M=Ga, Sc, In, Y, Gd, La)

J. Hermet, F. Bottin, **G. Dezanneau**, G. Geneste

Journal of Materials Chemistry A, 2, 460, **2014**

Oxygen diffusion mechanism in the mixed ion-electron conductor $NdBaCo_2O_{5+x}$

Y. Hu , O. Hernandez , T. Broux , M. Bahout , J. Hermet , A. Ottochian , C. Ritter , G. Geneste , **G. Dezanneau**

J. Materials Chemistry, *22*, 18744, **2012**

Simulations of $REBaCo_2O_{5.5}$ (RE=Gd, La, Y) cathode materials through energy minimisation and molecular dynamics

J. Hermet, B. Dupe, **G. Dezanneau**,

Solid State Ionics, *216*, 50-53, **2012**

Effects of biaxial strain on bulk 8% yttria-stabilised zirconia ion conduction through molecular dynamics

G. Dezanneau, J. Hermet, B. Dupe,

Int. J. Hydrogen Energy, *37(9)*, 8081-8086, **2012**