LAB & PEOPLE

- Name of the hosting lab: Laboratoire Chimie Electrochimie Moléculaire et Chimie Analytique, Laboratoire CEMCA UMR CNRS 6521.
  General activities of the lab: Chemistry, Synthesis, Mass Spectrometry and Electrochemistry analysis.
  Website: https://www.umr6521.cnrs.fr/
  Number of staff / PhD: 28 permanents, 10 PhD students
- Supervisor name and contact: Alexandre Lebon, alexandre.lebon@univ-brest.fr

TOPIC OF THE INTERSHIP

- Scientific context of the internship (max 20 lines)

Hydride materials like those using magnesium, are appealing for hydrogen storage applications [1]. For instance, MgH_2 one of the most promising hydride for thermal energy storage offers an energy density significantly higher than that of molten salt-based heat storage [2] and that could be used after a cell concentrating the solar power. The hydride MgH_2 diplays a relative weight of H with respect to the total system (storage gravimetric capacity) of 7.7 %. However its use in technological applications within a solid tank in light duty hydrogen vehicle is hindered due to the initial hydrogenation of the metal (activation) requiring more than 300°C and hundreds of bars of pressure [3]. In fact, the strong binding between H and Mg lowers the adsorption-desorption kinetics and despite a high enough storage gravimetric capacity, the deliverable capacity is too low. Elemental substitution with other metals were proposed to circumvent the aforementioned drawbacks. Zinc enters in the composition of magnesium-based alloys for which mechanical treatments [4] were shown to favor the activation process and was also shown theoretically as a good substituent to weaken the Mg-H bond [5].
We propose to build Mg-rich nanoparticles of Zn-Mg and investigate their propensity to capture hydrogen [6,7] either within the nanoparticles (absorption) or at the surface (adsorption). The dissociation of molecular hydrogen at the surface will be examined as well as the possible pathways of the proton towards the core of the nanoparticles.

Keywords DFT simulations, Magnesium based alloys, Nanoparticles, Hydrogen insertion

Bibliography:

[1] M. S. Salman *et al.*, "The power of multifunctional metal hydrides: A key enabler beyond hydrogen storage", J. Alloys Compd 920 (2022) 165936.
[2] D.N. Harries *et al.*, " Concentrating solar thermal heat using metal hydrides", Proc. I.E.E.E. 100 (2012) 539.
[3] A.A.C. Asselli *et al.*,"The role of morphology and severe plastic deformation on the hydrogen storage properties of magnesium", Int. J. Hydrog. Energy 39 (2014) 12778.
[4] A.A.C. Asselli *et al.*,"Effects of equal-channel angular pressing and accumulative roll-bonding on hydrogen storage properties of a commercial ZK60 magnesium alloy", Int. J. Hydrog. Energy 40 (2015) 16971.
[5] R. Varunaa *et al.*, "Zinc substituted MgH_2-a potential material for hydrogen storage applications", Int. J. Hydrog. Energy 44 (2019) 13632.
[6] Nanoscale reactivity of Zn_xMg_{20-x} clusters investigated by structural and electronic indicators, A. Lebon, A. Aguado, A. Vega, Corrosion Science 124 35-45 (2017)
[7] Why are Zn rich Zn-Mg rich nanoalloys optimal protective coatings against corrosion? A first principle study of the initial stages of the oxidation process. P. Alvarez-Zapatero, A. Lebon, R. H.

Aguilera del Toro, A. Aguado and A. Vega, Physical Chemistry Chemical Physics 23(43) 24685 (2021)

- Tasks and duties entrusted to the student:
  1. Finding putative global minima for Mg-rich MgZn nanoalloys.
  2. Test the structures with DFT simulations codes (siesta or VASP).
  3. Test H absorption and adsorption.

- Skills to be acquired or developed:
  1. Acquire experience with DFT computations, a microscopic method of analysis.
  2. Learn about the electronic indicator of reactivity
  3. Extraction of data

PROFILE OF THE DESIRED STUDENT

- Minimum level of study required: Master 1, Master 2 Student
- Field(s) of study: Electronic Structure Calculations, Computer Science
- Scientific skills: Solid State Physics, a programming language: C, Fortran or Python
- Language skills required: fluent in english or spanish

THE INTERNSHIP ASSIGNMENT:

Desired duration of the internship (in months): 4
Desired Starting date of the mission: march-april 2023
Indicative weekly schedule: *35h / week*
Remuneration: 600€/month, paid on French SEA-EU funds for a maximum of 5 months; additional Erasmus grant could be asked to your own university.

Internship agreement: *an internship agreement will be signed.*

To SEA-EU students:
If you're interested please send your CV and letter of motivation to the scientist in charge, ***email: alexandre.lebon@univ-brest.fr before the 15/ 02/ 2023.***