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Doctoral project in Metz and Nancy (France)

Hydrogen storage mechanisms in MAX phases

Simulations and experiments

The doctoral researcher will be part of the team for the H2MAX project (*Hydrogen storage mechanisms in MAX phases*), which is funded by the region Grand-Est over 36 months.

This doctoral project aims to advance the understanding of how the chemistry of the A and M elements and crystalline defects influence hydrogen (H) storage mechanisms in MAX phases and their two-dimensional derivatives, the MXenes.

MAX phases are layered hexagonal carbides and nitrides with the general formula $M_{n+1}AX_n$ (n = 1–3), where M is an early transition metal, A is a group IIIA or IVA element (e.g., Al or Si), and X is carbon and/or nitrogen. These materials combine metallic and ceramic properties, including high electrical and thermal conductivity, machinability, and damage tolerance. MXenes are obtained by selective etching of the A layers from MAX phases, yielding 2D materials ($M_{n+1}X_nT_x$) with high surface areas, tunable chemistries, and promising properties for energy storage and catalysis, including hydrogen storage.

The project focuses on various MAX phases (Ti_3AlC_2, Ti_3SiC_2, Ti_2AlC, Ti_2SiC, V_3AlC_2, V_2AlC) and corresponding MXenes (Ti_3C_2, Ti_2C, V_3C_2, V_2C). These systems were selected for their relevance to H storage and their availability via synthesis, enabling direct comparison with *ab initio* simulations. This integrated approach, made possible by prior work, is key to bridging experimental and theoretical insights.

Experiments will use tools available at LEM3: hydrogen uptake and kinetics will be measured with a Sievert apparatus, while microstructures will be characterized before and after hydrogenation using the MICROMAT platform. On the modeling side, *ab initio* calculations will be performed using VASP on the EXPLOR mesocenter and national HPC facilities. H insertion and migration energies will be computed in both pristine and defected structures to identify the key mechanisms involved.

In addition, the development of a machine learning (ML) potential based on the project's results may be pursued to model more complex systems beyond the reach of *ab initio* methods—such as dislocation-H interactions or Mg-MAX interfaces, toward realistic Mg-MAX nanocomposites.

This project is inherently interdisciplinary, as it requires the doctoral researcher to develop and apply advanced skills in both experimentation and numerical simulation. This dual expertise will allow doctoral researcher not only to gain deep insight into the phenomena under investigation but also to master a wide range of methodologies and analytical tools recognized in both academic and industrial settings. As such, the doctoral researcher will be well-positioned to integrate into the job market and pursue high-value positions upon completion of the PhD.

Recommended readings:

- M.W. Barsoum, T. El-Raghy, *American Scientist*, Vol. 89, No. 4 (2001), pp. 334-343 (https://www.jstor.org/stable/27857502)
- Y. Gogotsi, and B. Anasori, ACS Nano, Vol. 13 (2019), pp. 8491−8494 (https://doi.org/10.1007/s41127-022-00053-z)
- V. Bérubé, G. Radtke, M. Dresselhaus, G. Chen, *International Journal of Energy Research*, Vol. 31 (2007), pp. 637-663 (https://doi.org/10.1002/er.1284)

Your skills

The following qualifications are required:

- Master's degree in materials science or a closely related field (e.g., quantum/statistical physics or nanoscience)
- Solid understanding of materials science and condensed matter physics.

The following qualifications are beneficial:

- **Modeling skills:** Prior experience or strong interest in simulations and computational modeling of materials behavior. Experience with programming languages such as Python is a plus.
- **Characterization techniques:** Knowledge of microstructural characterization, particularly using electron microscopy techniques (e.g., SEM, TEM, EBSD).

We offer

A 36-month full-time PhD position is available. The doctoral contract is ideally set to begin on October 1, 2025, with some flexibility for an earlier or later start. The position includes health coverage and paid holidays. It offers a dynamic international research environment and close supervision by experienced senior scientists. The gross monthly salary is approximately €2,200.

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The doctoral school:

As a PhD student, you will be enrolled at Université de Lorraine and affiliated with the C2MP doctoral school (***C**himie, **M**écanique, **M**atériaux, **P**hysique*: Chemistry, Mechanics, Materials, Physics). You will have the opportunity to benefit from a wide range of training programs and professional development courses throughout your PhD.

The supervision team:

Dr. Lucile DEZERALD, Tenured Associate Professor at Université de Lorraine (France), expert in materials physics and simulations [https://materiaux.cnrs.fr/lucile.dezerald/].
Prof. Antoine GUITTON, Full Professor at Université de Lorraine (France) & Adjunct Professor at Georgia Institute of Technology school of Materials Science and Engineering (USA), expert in materials science [www.antoine-guitton.fr].

About the host laboratories:

The LEM3 (Laboratory for the Study of Microstructures and Mechanics of Materials) in Metz and the IJL (Jean Lamour Institute) in Nancy are two of France's leading research centers in materials science and engineering. Both are joint units of Université de Lorraine and the CNRS, with strong industrial and international ties.

LEM3, where the doctoral researcher will be based, specializes in microstructures, mechanics, and materials processes, with expertise in plasticity, electron microscopy, multiscale modeling, and hydrogen storage, including dedicated facilities for microstructure optimization. IJL focuses on materials, surfaces, metallurgy, nanoscience, and electronics, and hosts advanced infrastructure such as cleanrooms and a unique ultra-high vacuum platform.

Located in the Grand-Est region near Germany and Luxembourg, LEM3 and IJL form a major hub for European research, bringing together over 800 scientists working at the interface of fundamental science and applied innovation in energy, health, mobility, and manufacturing.

Advantages of working at the Université de Lorraine:

As a valued member of our team, you will have access to the comprehensive social protection system in France, including:

- **Universal healthcare coverage:** France's public healthcare system provides broad coverage for medical expenses, including doctor visits, prescription medications, and hospital stays. As a PhD student affiliated with the Alsace-Moselle local regime, you will benefit from enhanced reimbursement rates—typically around 90% of standard medical costs.
- **Generous annual paid leave:** Generous annual paid leave: Take advantage of our generous annual leave policy, which allows you to take up to 45 days of annual leave to recharge and rejuvenate.
- **Retirement pensions:** You will contribute to the French retirement system and receive a pension upon reaching retirement age.
- **Unemployment benefits:** You may be eligible for unemployment benefits after your contract ends, depending on your situation and eligibility criteria.
- **Sickness benefits:** If you are ill or injured, you may be eligible for daily sickness benefits provided by the French Social Security system to partially compensate for lost income during your medical leave.
- **Maternity, paternity, and family leave:** You are entitled to take time off to care for your family and bond with your new child, in accordance with French labor and social protection laws.
- **Free education:** Public education in France is free for children from age 3 up to 18, although some additional costs (such as school supplies, meals, or extracurricular activities) may apply.
- **Personalized housing allowance:** Financial assistance is available in France to help individuals with modest incomes cover their housing costs. Eligibility and the amount granted depend on income, household composition, and the type of accommodation.
- **Participation in your public transportation subscription:** 50% of your public transportation subscription cost for commuting will be reimbursed by Université de Lorraine, in accordance with French labor law.
- **Opportunity for teaching:** You may have the opportunity to teach at Université de Lorraine, which comes with additional compensation for this responsibility.

How to apply?

Please send a detailed CV, a cover letter, and transcripts of your bachelor's and master's degrees **to the two email addresses listed in the header**. Recommendation letters are not required, but please include the contact details of your references.

Applications that are incomplete or missing the required documents may not be considered