

**JOB OFFER**

# PhD RESEARCHER

**Position: PhD researcher in atomistic simulations**  
**Offer date: CIIAE web**  
**Project: CIIAE – Ref. PD-ATOMÍSTICAS (HIDRÓGENO Y POWER-TO-X)**  
**Department: Hydrogen and Power-to-X**  
**Estimated starting date: 2023**

<b>Workplace:</b>	University of Extremadura. Cáceres campus	
<b>Tasks to be developed:</b>	<p>Atomistic simulations are a powerful tool to better understand the thermodynamics and kinetics behaviour of reactions which are important for energy conversion and storage. Advanced energy materials, such as catalysts and batteries, have complex atomic structures that defy modern characterization techniques. First-principles atomistic simulations shed light on the unexplored areas, thus providing key insights for future developments.</p> <p>The selected candidate is expected to perform the following tasks:</p> <ul style="list-style-type: none"> <li>– Creating atomistic simulations for various types of energy storage and hydrogen technologies</li> <li>– Collaborations with experimental researchers from CIIAE and beyond</li> <li>– Provide recommendations to decision makers based on modelling results</li> <li>– Writing 1 paper per year as first author or co-author in high-ranked journals</li> <li>– Project management and project administration (internal and external), also towards the CIIAE</li> </ul> <p>Challenges: In order to provide meaningful insights, first-principles atomistic simulations on advanced materials require experimental data from equally advanced characterization techniques. Besides, they require modern and powerful computational clusters (HPC) able to run novel libraries and software.</p>	
<b>Duration of the contract and salary:</b>	Temporary Contract Initial duration: September 2025, with the possibility of extension	Gross Salary + S.S. Fees Set by law
<b>Academic background required:</b>	Master's degree in materials science, chemistry, physics, engineering, mathematics, or related disciplines	
<b>Other education:</b>		
<b>Professional experience:</b>		
<b>Job requirements (have to be fulfilled):</b>	<b>Specific techniques (analytical, software, calculations, prototyping, etc.)</b>	<ul style="list-style-type: none"> <li>– Some first learning or working experience with computational modelling of materials or processes</li> <li>– Statistical skills, for example, statistical tests and regression</li> <li>– Knowledge of energy technologies including renewables, storage, hydrogen and power-to-X</li> </ul>

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	<b>Participation and/or collaboration in R&amp;D&amp;I/business projects</b>	
	<b>Languages</b>	Excellent oral and written skills in English
	<b>Cross-cutting competences</b>	<ul style="list-style-type: none"> <li>- Commitment to open science in terms of research methods, data and publications</li> <li>- Ability to work in a diverse and flexible academic environment in a team-oriented, but independent way</li> <li>-</li> </ul>
	<b>Willingness to travel and stay abroad</b>	The candidate is expected to travel, both nationally and internationally, in the context of projects and conferences
	<b>Publications: scientific articles (in journals indexed in Web of Science and/or Scopus), theses (PhD and/or Master's), presentations at conferences, reports, technical reports, technical guides, etc.</b>	A successfully completed master thesis on a relevant topic (completed or as-advanced-as-possible thesis to be included in the job application. The final, successful thesis will be required for starting with the position)
<b>To be evaluated (adds points to the final evaluation):</b> <ul style="list-style-type: none"> <li>- Some first learning or working experience with first principles, statistical learning models and machine learning.</li> <li>- Some first working or learning experience with VASP.</li> <li>- Knowledge of Spanish and/or Portuguese.</li> <li>- Experience with industrial collaborations and/or previous experience working on industry.</li> <li>- Average grade in master's and bachelor's degrees (documents to be included in the application).</li> <li>- Motivation letter (maximum 1 page) included in the application.</li> <li>- Evaluation provided by 2 referees via telephone conversation. The contact details of the referees (e-mail and telephone) are provided by the candidates in their application.</li> <li>- Master thesis (document to be included in the application)</li> </ul>		
<b>Selection process details:</b> <b>Technical test:</b> NO <b>Language (English):</b> yes ( <b>will be evaluated during the interview</b> ) <b>Job interview:</b> yes		

### Interested candidates:

Please, send all the documents requested by both the terms and conditions of the call for the proposal and the job offer, with the deadline being 15 calendar days from the day following the publication in the CIIAE web indicating the following reference: **Ref. PD-ATOMÍSTICAS**

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