

## JOB OFFER

# SENIOR RESEARCHER

**Position: Senior researcher in atomistic simulations**  
**Offer date: DOE publication**  
**Project: CIIAE - Ref<sup>a</sup> IS-ATOMÍSTICAS (HIDRÓGENO Y POWER-TO-X)**  
**Department: Hydrogen and Power-to-X**  
**Estimated starting date: January 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>– Developing an attractive research agenda in the field of atomistic simulations</li> <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>– Providing recommendations to decision makers based on modelling results</li> <li>– Acquisition of competitive funding, both private and/or public, e.g., PhD students and postdocs.</li> <li>– Successful Collaboration with universities, research institutes and companies at national and international level.</li> <li>– Successful guidance of PhD, postdocs and master students, i.e. they meet their own requirements</li> <li>– Writing publication as first author (e.g., 1 paper p.a. in a high-ranked journal)</li> <li>– Project management and project administration (internal and external), also towards the department and 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: November 2024, with the possibility of extension	Gross Salary + S.S. Fees Gross Salary Range: 41 000 € - 45 000 €
<b>Academic background required:</b>	Doctoral degree in materials science, chemistry, physics, engineering, mathematics, or related disciplines	
<b>Other education:</b>		
<b>Professional experience:</b>	<ul style="list-style-type: none"> <li>– At least 2 years of post-doctoral experience</li> <li>– Proven experience in acquiring and/or writing competitive project proposal, for example, project or career funding</li> </ul>	

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		<ul style="list-style-type: none"> <li>– Proven experience in supervising PhD and/or master students (for example, as daily supervisor)</li> </ul>
<b>Job requirements (have to be fulfilled):</b>	<b>Specific techniques (analytical, software, calculations, prototyping, etc.)</b>	<ul style="list-style-type: none"> <li>– Experience in first-principles computational modelling of materials relevant for hydrogen, storage and energy transformation</li> <li>– Experience in joint computational-experimental characterization of materials</li> <li>– Experience with VASP</li> <li>– Programming experience (any language)</li> <li>– Statistical skills, for example statistical tests and regression</li> <li>– Excellent analytical skills</li> </ul>
	<b>Participation and/or collaboration in R&amp;D&amp;I/ business projects</b>	Proven participation on at least 3 R&D projects
	<b>Languages</b>	Excellent oral and written skills in English
	<b>Cross-cutting competences</b>	<ul style="list-style-type: none"> <li>– Ability to lead a team towards financing and objectives</li> <li>– Commitment to open science in terms of research methods, data and publications</li> <li>– Proven experience with industrial collaborations and/or previous experience working on industry</li> <li>– Experience on collaborating with other colleagues from the same department and beyond</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>	Strong track-record of academic publications as first author and co-author as the candidate is expected to publish in top journals in the field. At least 10 publications in Scopus indexed journals.
<b>To be evaluated (adds points to the final evaluation):</b>		
<ul style="list-style-type: none"> <li>– Experience with statistical learning models and machine learning</li> <li>– More than 2 years of post-doc experience</li> <li>– Being the principal investigator of at least 1 project</li> <li>– Publications as last author</li> <li>– Knowledge of Spanish and/or Portuguese</li> <li>– Motivation letter (maximum 2 pages) included in the application.</li> <li>– Evaluation provided by 2 references via telephone conversation. The contact details of the references (e-mail and telephone) are provided by the candidates in their application.</li> </ul>		
<b>Selection process details:</b>		
<b>Technical test:</b> NO		
<b>Language (English):</b> yes (will be evaluated during the interview)		
<b>Job interview:</b> yes		

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### Interested candidates:

Please, send the curriculum vitae, with the deadline being 15 calendar days from the day following the publication in the DOE (Official Journal of Extremadura) indicating the following reference: **Ref<sup>a</sup> IS-ATOMÍSTICAS (HIDRÓGENO Y POWER-TO-X)**

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