



Reference: REQUIMTE 2025-19

Main research field: Chemistry

Sub research field: Theoretical and Computational Chemistry

1. In a meeting the Board of Directors of REQUIMTE has decided to open an international call for PhD holder Researchers, under a work contract for a non-fixed term. This announcement is intended to 1 (one) research position (**Reference REQUIMTE 2025-19**) to pursue scientific research activities in the project “SelfEnergyDriver – 3-in-1 Self-Powered Hybrid Energy-Driven Wearable Technologies: Unifying Energy Harvesting and Storage”, with reference 101171793, supported by European funds by European Research Council, in the field of Chemistry, with scientific subfields in Theoretical and Computational Chemistry, under a work contract for a non-fixed term, aiming at computational modeling using classical and *ab initio* molecular dynamics, as well as machine learning techniques, to predict the (electro)chemical properties of electrode materials and electrolytes, understand the phenomena and mechanisms of energy production and storage at electrode–electrolyte interfaces, design architectures, and predict the performance of self-powered hybrid devices.

2. Applicable Legislation

Decree-Law no. 57/2016 of August 29th, amended by Law 57/2017 and Regulatory Decree No. 11- A / 2017 which approved the doctorate hiring regime destined to stimulate scientific and technological employment for all knowledge areas (RJEC); Portuguese Labour Code, approved by Law 7/2009 of February 12, in its actual form.

3. Pursuant to article 13 of RJEC, the tender selection panel is formed by: Professor Doctor Clara Isabel Barbosa Rodrigues Pereira (Assistant Professor at the Faculty of Sciences of the University of Porto, Chair of the Jury by delegation of the Director of REQUIMTE), Professor Doctor Maria Natália Dias Soeiro Cordeiro (Associate Professor at the Faculty of Sciences of the University of Porto), and Professor Doctor João Paulo Cristovão Almeida Prates Ramalho (Associate Professor at the Chemistry and Biochemistry Department of the School of Science and Technology of the University of Évora).

4. The workplace shall be at Department of Chemistry and Biochemistry of the Faculty of Sciences of the University of Porto.

5. Monthly remuneration to be paid is the one set by article 23 (3) of RJEC, corresponding to level 33 of the Single Salary Table, approved by Order no. 1553-C/2008 of December 31st, i.e. 2.351,53 Euros.

6. Application can be submitted by any national, foreign and stateless candidate(s) holding a doctorate degree in Chemistry or related area and a scientific and professional curriculum whose profile is suited for the activity described below (item 7).

In case the doctorate degree was awarded by a foreign higher education institution, it must comply with the provisions of Decree-Law no. 341/2007 of October 12th, and all formalities established therein must be complied with at the signature of work contract.

7. The tender admission general requirements are those defined in the previous point 6, and additional specific requirements include experience in computational studies of materials at interfaces, namely in Molecular Dynamics calculations (both classical and *ab initio*), DFT calculations, as well as related software, and in machine learning techniques.

8. Pursuant to article 5 of RJEC, the selection is to be made based on the evaluation of the scientific and curricular career of the candidate.

9. Scientific and curricular career evaluation focuses on relevance, quality and up-to-datedness:

a) of scientific, technological, cultural or artistic production in the last five years, considered most relevant by the candidate;

b) of research activities, fundamental or applied science, developed in the last five years, considered of higher impact by the candidate;

c) of knowledge extension and dissemination activities developed in the last five years, namely under the scope of the promotion of culture and scientific practices, deemed most relevant by the candidate.

d) of activities of science management, technology and innovation programs, or of experience in observing and monitoring the scientific and technological system or higher education, in Portugal or abroad.

10. The five-year period mentioned above can be extended by the panel, if requested by the candidate, whenever the suspension of scientific activities is reasoned by socially protected grounds like paternity leave, long-term serious illness, and other legal situations of unavailability to work.

11. The **evaluation criteria** are the following:

The evaluation of the CV of the candidates, in particular the scientific merit and research experience, will take into consideration the elements presented for the last five years of activity falling within the scope of the specific areas of the tender indicated in Point 1 and the specific requirements outlined in point 7, according to the following criteria:

11.1 Integrated assessment of the curriculum trajectory of the candidate, based on an overview of their scientific merits, namely:

I. Overall scientific coherence of the CV – 15%;

II. Diversity and quality of scientific indicators in the specific areas indicated in the call, including relevant published peer-reviewed articles and scientific communications – 25%;

III. Participation in research projects and students supervision – 10%.

11.2 Relevant experience, proved in CV, in:

I. Materials modeling, particularly of electrodes, electrolytes, and their interfaces – 15%;

II. Use of software packages such as GROMACS (and/or LAMMPS), GAUSSIAN (and/or ORCA, GPAW, VASP), CP2K (and/or FHI-AIMS) – 10%;

III. Experience in the development of machine learning models – 15%;

IV. Programming experience in Python – 10%.

Only candidates who obtain a classification equal to or greater than 50% in the parameters indicated at points 11.1 and 11.2 will be eligible.

12. In the case of admitted candidates whose evaluation does not differ more than 10% from that obtained by the best positioned candidate, the jury will interview the best positioned candidate and the candidates in this situation. This will be aimed at obtaining clarifications and explanations about the curricular elements and additional information as well as to evaluate the attitude profile and motivation of the candidate.

The final score of each jury member is obtained by the following assessment: 90% scientific and curricular career evaluation and 10% interview.

13. Candidate final classification system shall be given based on a scale 0 to 100.

14. The panel shall deliberate by means of roll-call vote justified under adopted and disclosed selection criteria, with no abstentions allowed.

15. Minutes of panel meetings shall be executed and include a summary of all occurrences of said meeting, as well as of all votes casted by the members and respective reasoning, and shall be provided to candidates whenever required.

16. After selection criteria application, the panel shall prepare a sorted list of approved candidates and respective classification.

17. Panel's final decision shall be validated by the leader of the institution, who is also in charge of deciding about the hiring.

18. Application formalization:

18.1 The applications are formalized at the electronic address <https://www.requimte.com/> with following documents in a digital form, in PDF format:

- i) Curriculum vitae;
- ii) Motivational Letter;
- iii) Qualifications Certificate;
- iv) Other relevant documentation.

18.2. The documents referred to in points i) to iii) are mandatory.

18.3 The application period is from **27/03/2025 to 09/04/2025**.

19. All candidates who formalize their applications in an improper way or fail to prove the requirements imposed by this tender are excluded from admission. In case of doubt, the panel is entitled to request any candidate to present further documentation supporting their statements.

20. False statements provided by the candidates shall be punished by law.

21. Both admitted and excluded candidate list and final classification list shall be published at the address of REQUIMTE (Praça Coronel Pacheco nº 15-6º andar, Porto), in the website of the Institute and the selected candidate shall be notified by email.

22. Preliminary Hearing and Final Decision Deadline: After publication, all candidates have 10 working days to respond. Panel's final decisions are pronounced within a period of 90 working days, from response period deadline.

23. This tender is exclusively destined to fill this specify position and can be terminated at any time until approval of final candidate list, expiring with the respective occupation of said position.

24. Non-discrimination and equal access policy: REQUIMTE actively promotes a non-discrimination and equal access policy, wherefore no candidate can be privileged, benefited, impaired or deprived of any rights whatsoever, or be exempt of any duties based on their ancestry, age, sex, sexual preference, marital status, family and economic conditions, instruction, origin or social conditions, genetic heritage, reduced work capacity, disability, chronic illness, nationality, ethnic origin or race, origin territory, language, religion, political or ideological convictions and union membership.

25. The panel has approved this announcement in meeting held on 17th of March of 2025.

26. According to Decree-Law no. 29/2001 of 3 February, disabled candidates shall be preferred in a situation of equal classification, and said preference supersedes any legal preferences. Candidates must declare, on their honour, their respective disability degree, type of disability and communication/expression means to be used during selection period on their application form, under the regulations above.

27. The selection of candidate to be hired is determined by orientations and regulations issued by European Commission upon verification of all legal requirements. REQUIMTE is entitled to cancel the present process in case the legal requirements are not fulfilled.