Open post-doctoral research position in the ERC project REACHER

Topic of the open position:

Development of a procedure to search and design *reactive* working fluids for thermodynamic cycles

Place:	*Laboratoire de Réactions et Génie de Procédés (LRGP), 1 rue Grandville, 54000 Nancy, France.*
Duration:	*2 years.*
Starting period:	*April 2023 (flexible extension to September 2023).*

Deadline for application to the position: *28 February 2023*

Context of the project

With the aim to effectively increase the performance of power plants, refrigeration systems and heat pumps, the research project REACHER proposes the use of equilibrated reactive working fluids instead of inert ones. It applies an original methodology that integrates thermodynamic and kinetic predictive tools to discover and characterise suitable reactive fluids, allowing for the quantification of the effects of reaction features on system performance and optimal thermodynamic cycle architecture.

Objectives of the specific work

The postdoctoral researcher will develop an automatised procedure aimed to search and to design chemical reactions fulfilling specific thermodynamic and stoichiometric criteria. The reaction search will be done considering three databases own by the research team (DIPPR, DDB and NIST thermodynamic databases). Also, at least two reaction design methodologies used, to build molecules (dimers) being able to dissociate in their monomeric forms. The postdoc will also contribute to the environmental and safety characteristics of each of the found or design molecule taking part into the reaction.

Different computational tools will be used: Gaussian (for quantum chemistry simulations), molecular dynamic simulation programs (to be defined), artificial intelligence computational tools. Other programs will be added to the list if necessary.

Programming languages that will be used to build independent computational codes or to manage input/output files of other codes: Fortran, Python, Matlab.

Requested background knowledge

The development of the work described above requires a Chemical Engineering background, with a robust experience in computational programming. The expert knowledge in using at least Fortran, Python or Matlab is mandatory.

Tools and opportunities provided to the postdoc

The postdoc will be given with one computer or more, if needed. Also, licences to enable the use of databases or existing software's will be acquired if needed.

The postdoc will have the opportunity to participate to international conferences and all publications will be published in open access.

Finally, the postdoc being part of the scientific team of the ERC project REACHER, the collaboration with the members of the team will be necessary to guarantee a successful project and also important for the postdoc to develop team working skills.

To apply to this position, please send your:

- detailed CV,
- list of publications,
- and motivation letter

to the Principal Investigator of the project, Silvia LASALA, via the email silvia.lasala@univ-lorraine.fr.

For more information about the project and the current research team, see the website of the project: www.univ-lorraine.fr/erc-reacher.