1 postdoctoral position at the University of Namur on quantum chemistry simulations of surface-enhanced spectroscopy

Outstanding candidates are sought to work at UNamur (Namur, Belgium) in collaboration with the UCLouvain (Louvain-la-neuve, Belgium) on the SURFASCOPE project, focusing on the design and implementation of a numerical approach to interpret and guide Surface Enhanced Vibrational Spectroscopies (SEVS), based on second-principles calculations, i.e. on top of first-principles calculations (GAUSSIAN, ABINIT). Starting date is envisioned to be the 1st April 2023. The postdoctoral research project is joined to this announcement.

JOB REQUIREMENTS:

Highly motivated doctor in Chemistry, Physics or Materials Science with a solid background in *ab initio* simulations using atomic basis sets such as Gaussian, Dalton, turbomole, Knowledge of plane waves codes as well as having some coding experience (FORTRAN and/or Python) is a plus. Good knowledge of English, both written and oral, is compulsory.

ABOUT THE GROUP:

The retained candidates will join the group of V. Liégeois at the laboratory of theoretical chemistry of the UNamur. The SURFASCOPE is a collaborative project involving UCLouvain (X. Gonze and G.-M. Rignanese) and UNamur (L. Henrard and V. Liégeois), Belgium.

CONTRACT DETAILS:

The postdoctoral position is an 18-month contract. Salary follows the legal scale for postdoctoral positions in Belgium (indicatively around $3000 \in$). The candidate should be in situation of international mobility (not to have resided in Belgium more than 24 months in the last 3 years), and not have passed the PhD more than 6 years before the beginning of the stay.

HOW TO APPLY:

Applicants should send their CV (pdf) as well as a brief motivation letter and a brief description of their coding skills and scientific achievements, to <u>vincent.liegeois@unamur.be</u> before February 15, 2023. They should also arrange for two letters of recommendation to be sent to the same address. The candidates that have been selected upon their CV will be auditioned by videoconference during 30'.