

# Postdoc position in atomistic modelling of filled ices at extreme conditions at University of L'Aquila (Italy)

Applications are invited for a Postdoctoral position of 2 years at the University of L'Aquila, Italy.

The research project is a collaboration between theoretical (our group in collaboration with Prof. Sandro Scandolo at ICTP in Trieste and Profs. Andrea Zen and Dario Alfé at University Federico II in Naples) and high-pressure experimental groups in Italy (Rome, Florence and Camerino). Our task will be to develop multiscale atomistic simulation strategies to investigate the various phases of ice filled with gases and salts and water in contact with carbon based structures, to help our experimental collaborators to interpret their experiments and eventually to suggest new ones. Our approach will consist of generating a database of ab-initio data at the relevant physical conditions. The database will be fed to a Machine Learning algorithm that will generate a many-body potential energy surface for large-scale and long-time simulations.

**Details of the position:** The position is for 2 years (1+1). The net yearly salary, depending on the applicant's CV, is between about € 18.000 and € 33.000, paid in monthly installments. Preference will be given to candidates who are available and eligible to start the position before the end of 2023.

**Personal Specification:** We are looking for a skilled and highly motivated candidate with a solid background in Physics and Condensed Matter theory. Proven knowledge of Density Functional Theory and/or Machine Learning methods constitutes a clear advantage. Programming skills in Python and Fortran, as well as knowledge of high performance computing are considered a plus. Applicants must hold a PhD degree in Physics, Chemistry, Materials Science and Engineering or similar fields.

**Expression of Interest:** We encourage the interested candidates to send an expression of interest to Prof. Carlo Pierleoni ([carlo.pierleoni@univaq.it](mailto:carlo.pierleoni@univaq.it)) and Prof. Sandro Scandolo ([scandolo@ictp.it](mailto:scandolo@ictp.it)). Candidates should include a detailed CV containing a list of publications, a detailed description of both scientific and computational background and the name and email address of at least one referee who might be contacted for a letter of reference. The deadline for the expression of interest is November 15th, 2023.