Università degli Studi di Torino
Dipartimento di Chimica
Via P. Giuria, 7/9 10125 Torino, Italy

1 year Postdoctoral Position in *DFT and thermodynamic calculations for materials science*

- **ORGANISATION:** Università di Torino
- **RESEARCH FIELD:** Computational Materials Science
- **LOCATION:** Italy, Torino
- **TYPE OF CONTRACT:** Temporary
- **DURATION:** One year
- **JOB STATUS:** Full-time

Job description

The metallurgy group at the Dipartimento di Chimica, Università di Torino is looking for a postdoctoral researcher in the area of computational materials science. The research concerns the theoretical study of materials for energy applications (thermoelectrics, batteries, hydrogen storage) using Density Functional Theory (DFT) and computational thermodynamics. In details, the successful applicant will carry out one or more of the following tasks:

- calculation of transport properties in thermoelectric materials
- calculation of thermodynamic stability, phonons and activation energies for ion migrations in solid state electrolytes
- calculation of thermodynamic stability, including vibrational contributions, in hydrides
- simulations of phase transformations in the above materials using computational thermodynamics and the CALPHAD approach

Requirements

- The candidate should have a strong research expertise from at least one of these areas: density functional theory, computational thermodynamics, materials science modelling.
- The candidate should also be prepared to collaborate with faculty and students at the Department and at cooperating with other research groups at the Università di Torino.
- The successful applicant should have an outstanding publication record. Well developed analytical and problem-solving skills are required.
- We are looking for a strongly motivated person, who is able to work independently.
- Good command of English orally and in writing is required to present and publish research results.

Preferred qualifications

- A doctoral degree or an equivalent foreign degree, obtained within the last three years prior to the application deadline (With some exceptions for special reasons such as periods of sick or parental leave, kindly indicate if such reason exists in your resume).
- Previous experience with DFT calculations and VASP or Quantum Espresso codes.

- Previous experience in CALPHAD calculations

Supervisor: Prof. Mauro Palumbo, mauro.palumbo@unito.it

For info, available facilities and resources:
https://www.chemistry.unito.it/do/home.pl/View?doc=/research/Research_Chemistry_UniTo.html
https://www.chimica.unito.it/do/gruppi.pl/Show?_id=cpcf

For details, please contact: mauro.palumbo@unito.it

Applications will be accepted on-line at the following address:
https://www.unito.it/ricerca/fare-ricerca-unito/assegni-di-ricerca

Planned application deadline: June 2021 (check for updates at the above web address)