3-years PhD Position, Institute of Theoretical and Computational Physics, Graz University of Technology (Austria)

A three-years PhD position is available at the Institute for Theoretical and Computational Physics of the Graz University of Technology (Austria), to work on the project "Superhydra" (new high-pressure hydrides for superhydrogen storage and superconductivity), funded by the Austrian Science Fund FWF.



The goal of the project is to search for new high-temperature superconductors, investigating the high-pressure phase diagram of complex hydrides.

Two years ago, a record superconducting critical temperature (T_c) of 203 K was reported by the group of Mikhail Eremets (MPI Mainz) in a simple hydride (SH_3), demonstrating a new route to achieve high-temperature superconductivity, exploiting high pressures to amplify conventional pairing. In addition to being a record-holder, SH_3 was also the first example of a high- T_c

superconductor entirely predicted on a computer.

In contrast to simple hydrides, where the choice compounds is limited, complex (ternary or multinary hydrides) offer a larger flexibility, which can be exploited to optimize the superconducting properties. In our project, we will apply state-of-the-art *ab-initio* methods for superconductivity and material design (evolutionary algorithms, machine learning) to study the high-pressure phase diagram of these materials, which is mostly unexplored so far. The project will be carried out in close collaboration with Prof. Lilia Boeri (Dipartimento di Fisica, Sapienza Universita' di Roma), who is an expert on computational superconductivity, and with several high-pressure experimental groups.

What we are looking for: We are looking for a highly motivated student, with a master degree in physics, an excellent knowledge of theoretical condensed matter physics, programming and writing skills. A previous knowledge of DFT codes is an advantage, but not required. The working language is English, German is not required. To maintain our collaboration with the university of Rome, we expect the candidate to be willing to spend some time abroad and to travel to conferences and schools.

The starting date is flexible, between September 2017 and January 2018.

What we offer: The PhD position is paid according to Austrian salary rules (gross salary is 37 keuros/year), with all standard benefits, such as pension, health insurance, social security. The Graz University of Technology is an equal-opportunity employer.

- For information, visit the project website: https://superhydra.wordpress.com/ or CONTACT:
 - Prof. Wolfgang von der Linden, Institute for Theoretical and Computational Physics, TU Graz: mailto:vonderlinden@tugraz.at.
 - Prof. Lilia Boeri, Dipartimento di Fisica, Sapienza Universita' di Roma: lilia.boeri@uniroma1.it.
- > To APPLY, send a cover letter, a cv, and the name and contact of two possible references to: suphydrides@gmail.com. The deadline for applications is September 15, 2017.