Open PhD position

Applications are invited for a PhD position in the FWF-funded project
Transition Metal Chalcogenides under Extreme Pressures

About the project:
With respect to conventional superconductivity, a highly topical class of compounds being intensely investigated at the moment are van der Waals crystals, i.e., stacked materials whose sublayers are loosely held together by weak van der Waals forces. Prototypical examples for this class are the transition metal dichalcogenides, which are of particular interest with respect to superconductivity, due to the fact that their superconducting states coexist with, or appear in very close vicinity to charge-density wave phases. As the formation of both phases rests on strong electron-phonon coupling, these materials offer the exceptional opportunity to study the mutual influence of superconductivity and charge-density wave order.

In this project, we will employ evolutionary search methods to explore the high-pressure phase diagram of transition metal chalcogenides materials, with particular focus on identifying novel superconducting structures and phases close to lattice instabilities. A careful analysis of the electronic, vibrational, and electron-phonon coupling properties will allow us to describe the superconducting phases from first-principles. For dynamically unstable phases, we will determine whether the structure is likely to decompose completely, or transit to a charge-density wave phase.

Of special focus will be compounds where superconductivity and charge-density wave phases coexist, such as in the metallic transition metal dichalcogenides. Here, we want to achieve a detailed description of the superconducting phase within the charge-density wave completely from first-principles by calculating the superconducting gap function $\Delta_{\mathbf{k}}$ and critical temperature T_c. In addition, we envisage the *ab initio* determination of the critical temperature of the charge-density wave phase T_{CDW}. We will further investigate the effects of pressure on the electron-phonon coupling in these materials, and the consequences of strain and compression for the mutual interaction of superconductivity and charge-density wave.

The project will be conducted at the *Institute of Theoretical and Computational Physics* (*Graz University of Technology*) in collaboration with the experimental group of Dr. V. Struzhkin (*Carnegie Institution for Science, Washington D.C.*) and the theory groups of Prof. L. Boeri (*Sapienza University of Rome*) and Prof. E.R. Margine (*Binghamton University-SUNY, New York*).

Required qualifications and how to apply:
Candidates should have a Master or Diploma degree in Physics, an interest in the computational modeling of materials, and good practice in numerical methods, especially DFT methods, Matlab, and Fortran (or equivalent). To apply, send an informal email including a short letter of motivation, CV, and list of possible references to 'christoph.heil@tugraz.at' by the end of August at the latest.

Main contact:
Dr. Christoph Heil
Institute of Theoretical and Computational Physics
Graz University of Technology
christoph.heil@tugraz.at