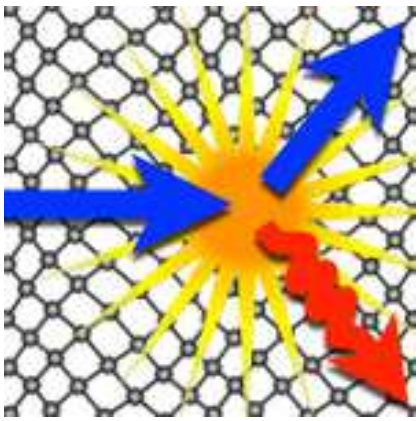
Master Thesis Projects in Computational Material Science

available at the Fritz Haber Institute of the Max Planck Society in Berlin



Master Thesis Projects (duration 25 weeks) are currently available for EPFL students in the *"Heat and Charge Transport"* group at the Theory Department (Prof. Matthias Scheffler) of the **Fritz Haber Institute of the Max Planck Society** in **Berlin**. The work of the *"Heat and Charge Transport"* group concerns methodological development, code development, as well as applications to accurately compute, understand, and predict transport properties of materials. The reliable assessment of the electronic structure and of the inter-atomic interactions by the means of *density-functional theory* (in its various approximations and advancements) represents the base of the research. On top of that, electronic-structure theory is used to investigate the thermodynamic and kinetic characteristics of materials, such as elastic constants, free energies, and vibrational properties, and more. *Ab initio molecular dynamics* plays a prominent role, given that it enables to reliably simulate the dynamics even at elevated temperatures, e.g., at and above 70% of the melting temperature, at which perturbative approaches would fail. With our methods we are able to accurately compute the *electron-phonon* and *phonon-phonon* coupling to all orders. This provides the route for the assessment of (electronic and vibrational) heat and charge transport phenomena.

Master Thesis Projects available to date span various topics that range from basic method development to the application of these methods to scientific and technological challenges in material science. For instance, applications include technologically relevant *high-temperature* materials such as Zirconia compounds, which are used in *thermal barrier coatings* which, for example, help to **improve fuel efficiency** of combustion engines Furthermore, we also investigate the charge and heat transfer properties of *thermoelectric materials*. Unraveling the electronic and atomistic mechanisms that determine the thermoelectric efficiency of these materials is key to the development of novel and improved ***waste-heat recovery*** *devices* that would enable a more sustainable energy economy.

Successful applicants should have a strong background in **theoretical solid-state physics**. Interest and experience in computer code development is highly desirable.

For more information, please contact:

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