

# Heidelberg Institute for Theoretical Studies

Think beyond the limits!

The [Heidelberg Institute for Theoretical Studies \(HITS\)](#) was established in 2010 by physicist and SAP co-founder Klaus Tschira (1940-2015) and the Klaus Tschira Foundation as a private, non-profit research institute. HITS conducts basic research in the natural, mathematical, and computer sciences. Major research directions at HITS include complex simulations across scales, data science and analysis, and enabling software and tools. Application areas range from molecules to stars, and from words to weather. An essential characteristic of the Institute is interdisciplinarity, implemented in numerous cross-group and cross-disciplinary projects. The base funding of HITS is provided by the Klaus Tschira Foundation.

The [Computational Carbon Chemistry \(CCC\)](#) group at the Heidelberg Institute for Theoretical Studies (HITS gGmbH) is looking to fill a

## PhD position (m/f/d) in computational chemistry

to work on the **ERC Starting Grant “PATTERNCHEM: Shape and Topology as Descriptors of Chemical and Physical Properties in Functional Organic Materials”**.

### Your role

Your interdisciplinary research project will involve high-level, high-throughput, and multiscale simulations of functional organic materials, including graphene derivatives, covalent organic frameworks, and hyperbranched polymers. You will also be developing and implementing novel representations of material structure and descriptors of the non-covalent interactions between materials and small molecules for machine learning. The ultimate goal of PATTERNCHEM is to build an all-encompassing, adaptable framework for modelling interactions of multifaceted functional organic materials with their molecular targets, filling the missing links with newly devised structural fingerprints and energetic descriptors.

### What qualifies you for this job

Successful candidates should have a Master's degree (or be close to completion) in chemistry, physics, materials science, or a related discipline, and an experience in chemical modelling and numerical simulations.



## The environment of this job

You will work in a dynamic research group, led by Dr. Ganna (Anya) Gryn'ova. You will be based at the Heidelberg Institute for Theoretical Studies, where you will find first-class research environment and outstanding computational infrastructure in a beautiful green setting on the banks of the Neckar River.

## We offer:

- An international und thriving work environment.
- Extensive social benefits, such as:
  - Subsidized cafeteria meals
  - Job ticket
  - Allowance for further training and career development
  - Company pension plan and additional health care benefits
  - 30 days of paid vacation
  - Family-friendly working environment

Learn more about [Working at HITS](#).

## To apply

Please submit the following documents

- Cover letter indicating earliest starting date
- Curriculum vitae including a publications list
- Relevant Certificates/Diplomas
- Contact details of two referees

via the following link <https://hits-ggmbh.jobs.personio.de/job/881622?language=en#apply>.

**Application deadline:** 31 December 2022. The starting date is negotiable.

For any additional information regarding the position please contact [Dr. Ganna \(Anya\) Gryn'ova](#).

HITS gGmbH stands for equal opportunities and we strongly believe that our research benefits from inclusive and diverse teams.