PhD positions (m/f/d) in data-enhanced molecular modelling in Heidelberg and Karlsruhe

Openings for PhD students in SIMPLAIX – a new Strategic Research Initiative between the Heidelberg Institute for Theoretical Studies (HITS gGmbH), Heidelberg University and Karlsruhe Institute of Technology (KIT). SIMPLAIX is an interdisciplinary cooperation focused on bridging scales in modeling molecules and molecular materials by combining machine learning and multiscale simulation-based approaches.

You will work in a dynamic, highly interdisciplinary research environment in close collaboration with other SIMPLAIX members. You will be based at one of the participating research institutions, where you will find a first-class research environment and will have access to outstanding computational infrastructure.
We are looking for highly motivated scientists to join one of the four collaborative projects. Details of each project are listed below. Applicants should have a master's degree in chemistry, physics, mathematics or a related discipline, and experience in either molecular modelling, numerical simulation, or machine learning. The deadline for applications is 15.02.2022.

Project 2 (at KIT):
Excited states potential energy surfaces and spin flips
This project focuses on the excited states properties of (bio)molecules and organic materials. Combined QM/MM calculations will be applied using high level quantum chemistry and semi-empirical methods. To improve and accelerate the calculations, machine-learning methods, like regression and neural networks, will be applied. This joint project of the labs of Marcus Elstner and Patrick Friederich (KIT) and Andreas Dreuw (Heidelberg University)
Candidates must have experience in molecular dynamics simulation, quantum mechanical calculations and modeling of biomolecular structures. For details on how to apply, see; https://www.pse.kit.edu/karriere/joboffer.php?id=30695&new=true&language=en

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Project 4 (at Heidelberg University):
Representations and machine learning for molecular systems.
Just which representation is best suited to make predictions about conformations, dynamics and other molecular properties is an open question as is the question how to best represent long-range interactions in machine learning models of molecular systems. In this joint project between the labs of Fred Hamprecht and Pascal Friederich (KIT), we will try to find answers to these fundamental questions. Candidates must have demonstrated successful foundational methods development in machine learning, quantum chemistry, optimization or another relevant field.
To apply, please send full details including your BSc and MSc thesis and pointers to any code you may have developed to fred.hamprecht@iwr.uni-heidelberg.de

Project 6 (at HITS):
Machine learning for supported organic electrode materials.
In this project, we aim to develop a screening and design framework for graphene-based nanocomposites as organic electrode materials for rechargeable batteries by combining high-level quantum-chemical computations, high-throughput screening, and machine learning techniques. You will work primarily in the Computational Carbon Chemistry (CCC) group, led by Ganna Gryn'ova and based at HITS; you will closely collaborate with the groups of Pascal Friederich and Marcus Elstner at KIT.
For details on the position and on how to apply, submit your application via the HITS website

Project 8 (at HITS):
Learning molecular bond rupture.
This project lies at the interface of mechanochemistry and machine learning and aims at predicting the weakest bond in a molecule or molecular material under tension. You will develop a novel scale-bridging approach based on quantum chemistry, molecular dynamics simulations, and neural networks, and apply it to a biological problem of high relevance. You will be primarily based in the Molecular Biomechanics (MBM) group led by Frauke Graeter at HITS, and will closely collaborate with the Andreas Dreuw, Ganna Gryn'ova and Pascal Friederich groups in SIMPLAIX.
For details on the position and on how to apply, submit your application via the HITS website