

## SIMPLAIX: “magic triangle” advancing molecular research

“SIMPLAIX” has officially started: In this new collaboration, researchers from HITS, Heidelberg University, and Karlsruhe Institute of Technology



(KIT) pool their expertise in machine learning to address challenges in the computer simulation of biomolecules and molecular materials. The collaboration is enabled by the Klaus Tschira Foundation. On 12 April 2022, the SIMPLAIX inaugural symposium took place at the Studio Villa Bosch in Heidelberg, with project members and representatives of all three institutions participating. In this hybrid meeting, 45 partici-

pants attended the event in person, another 30 people joined via videoconference.

### Finding new approaches to molecular design

“SIMPLAIX will enable us to collaborate on interdisciplinary, interinstitutional research projects”, said SIMPLAIX spokesperson **Rebecca Wade** (HITS), who chaired the event and gave an introduction to the structural and scientific aspects of the collaboration. “By combining machine learning and simulation approaches, we expect to gain novel insights into scale-bridging molecular phenomena in complex biomolecules and molecular materials that will ultimately lead to new approaches to molecular design.”

Welcome addresses by Carsten Könneker (Managing Director, Klaus Tschira Foundation), **Frauke Gräter** (Scientific Director, HITS and SIMPLAIX co-spokesperson), Oliver Kraft (Vice President for Research, Karlsruhe Institute of Technology), and Matthias Weidemüller (Vice-Rector for Innovation and Transfer, Heidelberg University) emphasized the importance and the impact of this initiative.



„SIMPLAIX fits perfectly with the aims of the Klaus Tschira Foundation”, Carsten Könneker remarked, “since we firstly facilitate top research, secondly, we support young researchers, and thirdly, we foster interdisciplinarity. SIMPLAIX combines all three. So we are very much looking forward to all the synergies this magic triangle offers.”

Finally, two members of the newly established SIMPLAIX international scientific advisory board - both experts in machine learning approaches for studying molecular systems - gave scientific talks: Anatole von Lilienfeld (University of Vienna) talked about “Quantum Machine Learning”, and Jörg Behler (University of Göttingen) explained “High-dimensional neural network potentials for simulations of complex systems”.



### Via Data

The HITS blog can be found on the “Scilogs” portal at <https://scilogs.spektrum.de/via-data/>.

## HITS

### Anna Wienhard elected to the European Academy of Science



HITS group leader **Anna Wienhard** (GRG) has been elected to the European Academy of Science (EURASC). The

EURASC is a non-profit non-governmental, independent organization of the most

distinguished scholars and engineers performing forefront research and the development of advanced technologies, united by a commitment to promoting science and technology and their essential roles in fostering social and economic development.

### HITS group leader member of online journal editorial board

**Ganna Gryn'ova**, head of the CCC group at HITS, is a new Early Career Advisory Board member of the journal *Helvetica Chimica*



Acta. The journal publishes high-quality research from all fields of chemical sciences in monthly issues. Since the re-launch in 2017, *Helvetica* has been published in an on-line-only format.

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### New employees and visiting scientists

#### Master's students:

#### Student scholarships:

#### Pre-docs:

#### Post-docs and research associates:

#### Visiting scientists:

#### Klaus Tschira Guest Professor:

Melanie Käser (MCM)

Anastasiia Nihei (CCC), Solomiya Serkiz (AIN)

Rostislav Fedorov (CCC), Jiajun Shi (GRG)

Haitham Abaza (SDBV)

Helman Amaya-Espinosa, Mikaela Farrugia, Juan David Orjuela Zuniga (all MBM)

Antonis Rokas (Vanderbilt University, USA)

**HITS groups 06/2022:** *Astroinformatics (AIN), Computational Carbon Chemistry (CCC), Computational Molecular Evolution (CME), Computational Statistics (CST), Data Mining and Uncertainty Quantification (DMQ), Groups and Geometry (GRG), Molecular Biomechanics (MBM), Molecular and Cellular Modeling (MCM), Natural Language Processing (NLP), Physics of Stellar Objects (PSO), Scientific Databases and Visualization (SDBV), Stellar Evolution Theory (SET), Theory and Observations of Stars (TOS).*

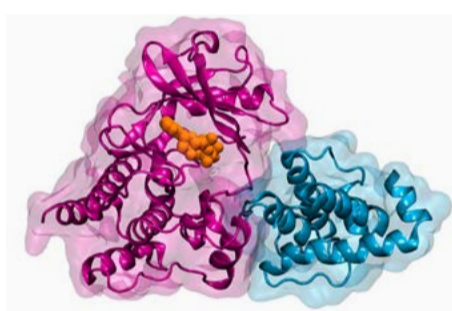
## HITSters

### “Something in the way they move” – zooming in on cell migration

Getting from A to B can be a tricky business, especially for cells on the move. An international team of researchers from HITS and the University of Helsinki have zoomed in on the biochemical and biomechanical processes underlying cell migration by taking a closer look at one of the major players, the pseudokinase ILK. The results of their study, published in the Proceedings of the National Academy of Sciences (PNAS), improve our understanding of this intriguing protein.

While the vast majority of cells stay roughly where they are during their lifetime and only travel short distances, there are a few specialized cells which need to move freely and quickly to fulfill their tasks. But whether fast or slow, inert or agile, they need to find the right balance between structural stability and flexibility by sensing and responding to a broad variety of biochemical and mechanical signals from their neighboring cells and the matrix to which they adhere.

Large protein complexes mediate this signal transduction between the cell and the matrix. One crucial protein in this complex



is integrin-linked kinase (ILK). “As a pseudokinase, ILK is not capable to catalyze a chemical reaction, as conventional kinases do,” says first author **Isabel Martin** from the “Molecular Biomechanics” group (MBM) at HITS. “It was therefore interesting to us why ILK still binds ATP, the small molecule normally used for catalysis, and how that relates to cell motion.”

By combining molecular dynamics simulations with cell biology involving traction force microscopy – the latter two carried out by colleagues at the University of Helsinki – the HITS researchers investigated the role of ATP-binding to human ILK, and examined the altered kinase dynamics and cell behavior as a result of ATP removal. “Only by using simulations, we could analyze ILK in molecular detail, and were able to see that ATP gives structural stability to

ILK. This effect is the result of an internal force propagation pathway from ATP to residues that bind an important adaptor protein,” Martin says. “Our idea now is that ATP in ILK adopted a new and unforeseen function, namely, to aid ILK to relay mechanical forces by giving it structural stability.” In a further step they verified the predictions from the simulations and moved beyond their time- and length scales to study the large-scale cellular effects of retained ATP-binding to ILK, for which they joined forces with colleagues in Finland.

The surprise was that ATP here does not carry its conventional biochemical role, but is a mechanical stabilizer – a small molecule making a big difference. And **Frauke Gräter**, head of the MBM group at HITS and co-author of the study, summarizes: “Our findings add another piece in the puzzle to improve our understanding of how cells can stay where they are supposed to but move when they are required to.”

*Isabel M. Martin, Michele M. Nava, Sara A. Wickström, and Frauke Gräter: ATP allosterically stabilizes integrin-linked kinase for efficient force generation. PNAS, Vol. 119 | No. 11. <https://www.pnas.org/doi/10.1073/pnas.2106098119>*

## Research

### Beyond the limits: HITS helps Ukrainian researchers

On 24 February 2022, Russia invaded Ukraine and has caused a humanitarian catastrophe.

We at HITS have been concerned about the safety and well-being of the people there ever since, also for very personal reasons, as some of our researchers have family and friends in Ukraine.

We are particularly concerned about our colleagues at Ukrainian universities and other academic institutions. The catastrophic effects of the war on many displaced students and researchers were foreseeable right from the start.

That is why we decided at the beginning of March to advertise positions for students and researchers from Ukrainian universities in a total of eight research groups at HITS, ranging from internships to residencies for visiting scientists.

Since then, the HITS Human Resources Department has received numerous inquir-



ries. Sometimes the expertise and professional qualification of the applications could not be reconciled with the very specialized research fields of the Institute, but scholarships were approved for two Ukrainian young female scientists at HITS: **Solomyia Serkiz** has been affiliated to the Astroinformatics Group (AIN) since April, and **Anasta-**

**sia Nihei** to the Computational Carbon Chemistry Group (CCC) since June.

In addition, HITSters informed the public about the events in Ukraine and related activities at HITS. Scientific Director **Frauke Gräter** explained the groups' relief efforts in a radio interview for “Campus Report.”

Group leader **Ganna Gryn'ova** (CCC), who is Ukrainian and helped her mother to escape, also gave a radio interview and described her very personal experiences with the war, the demonstrations and the propaganda. PhD student **Kiril Maltsev** (PSO, HITS Lab), who has roots in both Ukraine and Russia, talked about how different the information is that his friends and family receive in each country, and what can be done about disinformation. Regardless of how the situation in Ukraine unfolds: HITS will continue to help and support wherever this is possible.

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## Beyond the limits



# The Charts