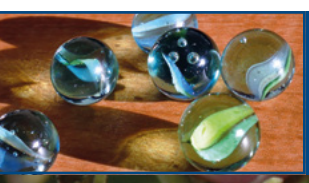
Carbon chemistry at HITS: Tremendous potential

Dr. Ganna Gryn'ova is set to lead the new junior group Computational Carbon Chemistry (CCC) at HITS, which will launch in April 2019. The group will use state-of-the-art computational chemistry to explore and exploit organic materials while focusing on graphene-based materials due to the many advantages they maintain over their conventional inorganic counterparts. In addition to being biocompatible (i.e., less harmful to the environment), graphene-based materials are extremely variable in their structures, mechanically flexible, and have unique electronic and optical properties. The group will develop computer-based tools and concepts for designing and screening new graphene-based materials and devices with target applications in metal-free catalysis and molecular electronics. Research topics will include the degradation of environmental pollutants, developing the concept of catalysis inside molecular junctions, designing molecular sensors for environmental pollutants, and designing spin-polarized molecular junctions with graphene electrodes.

Ganna Gryn'ova studied chemistry at the Oles Honchar National University Dnipro, Ukraine, before pursuing a PhD in computational chemistry at the Australian National University, Canberra. She also conducted postdoctoral research at École polytechnique fédérale de Lausanne, Switzerland. In 2016, Ganna Gryn'ova was awarded the Marie Skłodowska-Curie Actions Individual Fellowship by the European Commission. "We are very happy to welcome Ganna as a new junior group leader," HITS Scientific Director Dr. Wolfgang Müller declared. "She is a distinguished researcher in a tremendously exciting field and an excellent communicator." As of April 2019, 11 research groups will be active at HITS.



HITS@Explore Science 2019: All about "Time" – This year, HITS will once again participate in the "Explore Science" event in the Luisenpark, Mannheim. From 22–26 May 2019, HITSters from the groups of Data Mining and Uncertainty Quantification (DMQ), Molecular and Cellular Modeling (MCM), and Molecular Biomechanics (MBM) will present hands-on stations on the topic of "Time."

HITS

HITSter becomes new editor of Monthly Weather Review

As of January 2019, **Dr. Sebastian Lerch**, a member of the Computational Statistics group (CST) at HITS and a mathematician by training, is associate member of the editorial board of Monthly Weather Review, a leading atmospheric science journal published by the American Meteorological Society. "Sebastian completed his PhD just two years ago," CST group leader **Prof. Dr. Tilmann Gneiting** declared. "This reflects the success of our efforts to create a supportive, interdisciplinary research environment for young scientists beginning their careers at HITS."

Gräter and Strube to become Marsilius Fellows at Heidelberg University

HITS group leaders **Prof. Dr. Frauke Gräter** (MBM) and **Prof. Dr. Michael Strube** (NLP) have been named Fellows of the Marsilius Kolleg of Heidelberg University from April 2019 until March 2020. Together with professor of English philology Vera Nünning, they will investigate whether a scientific article that is easy and enjoyable to read and that contains stylistic features that attract readers' attention is in fact read and cited more often than other articles. The Marsilius Kolleg of Heidelberg University bridges the gap between the sciences and humanities. Meetings and joint projects promote understanding and collaboration between the disciplines. "This interdisciplinary approach harmonizes perfectly with our motto 'Think Beyond the Limits!'" said HITS Scientific Director **Dr. Wolfgang Müller**.

New employees and visiting scientists

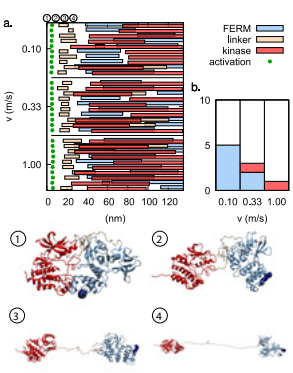
CCC: Dr. Ganna Gryn'ova, group leader; **CME:** Paula Breitling, master's student;
Communications: Angela Michel, employee; **DMQ:** Jiawei Zhang, visiting scientist;
ITS: Christian Zimmermann, employee; **MBM:** Paula Weidemüller, master's student;
MCM: Lorenzo Fabbri, master's student / Philip Ullmann, bachelor's student;
NLP: Haixia Chai, PhD student/fellow; **PSO:** Dr. Róbert Andrássy, Postdoc

HITS groups (04/2019)
Astroinformatics (AIN), Computational Carbon Chemistry (CCC), 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 Computing (SCO), Scientific Databases and Visualization (SDBV).

HITSTERS

"PINK": A cool tool for astronomy

The Astroinformatics group (AIN) helps astronomers to better analyze rapidly growing datasets with modern methods from computer science via digital tools that can be used easily. One of these tools is "PINK," the centerpiece of an explorative method used to analyze large and complex structured datasets. This tool supports astronomers in the analysis of the galaxy morphology in the radio wavelength regime. "PINK" (an acronym for Parallelized rotation and flipping INvariant Kohonen maps) was developed by group leader **Dr. Kai Polsterer** and his team together with **Dr. Bernd Doser** from the IT Services group. Recently, a new version was released. The software tool is now being used as an analysis tool by the precursors of the Square Kilometer Array (SKA) telescopes in Africa and Australia. Moreover, the method is also being used in the Low Frequency Array (LOFAR), a supercomputer-driven radio telescope. Source: https://github.com/HITS-AIN/PINK



A force for activation

In order to develop strategies for active tumor metastasis prevention, it is necessary to clarify the underlying activation process. Focal adhesion kinase (FAK) is a key enzyme involved in the signaling cascade of cancer invasion and metastasis and is thus a promising target for cancer therapeutics. HITS group leader **Prof. Dr. Frauke Gräter** (Molecular Biomechanics) and her team shed light on the force-mediated activation process of FAK together with colleagues from the LMU Munich and the Spanish National Cancer Research Centre (CNIO) in Madrid. Their study was published in the Proceedings of the National Academy of Sciences of the Unites States of America (PNAS).

A signaling protein, FAK regulates the essential processes of a cell: adhesion, migration, and survival. It is localized at the cytoplasmic site of focal adhesion complexes, which represents the feet of the cells. In the non-active state, FAK is auto-inhibited and inactive, with the active center hidden by a protein lid. HITS researchers examined whether mechanical force can open this lid and thereby trigger the activation of this key player by inducing conformational changes.

Frauke Gräter and her group simulated this process on high-performance computers to obtain a fully dynamic view of the events. "We successfully uncovered key steps in FAK activation in great detail," Frauke Gräter stated. "We were able to show that this signaling protein not only becomes activated by force but also stays active while being further stretched out." This fundamental insight into the mechanisms of a key enzyme in cancer development opens new pathways for future tumor therapy strategies.

Structural and mechanistic insights into mechanoactivation of Focal Adhesion Kinase. Bauer MS, Baumann F, Daday C, Redondo P, Durner E, Jobst MA, Milles LF, Mercadante D, Pippig DA, Gaub HE, Gräter F, Lietha D. PNAS, 2019, doi 10.1073/pnas.1820567116. Nature Communications-volume 9, Article number: 3325 (2018)

RESEARCH

Kerstin Hoppenhaus: "I've learned a lot about data."

Kerstin Hoppenhaus knows a thing or two about timing. She answers the phone after the second ring: "In ten minutes, I have to leave for an interview." Now, three months after the end of her stay as "Journalist in Residence" at HITS, the science journalist has long since returned to everyday life. "I'm working on a story about genetic resources and the endangered "wild" relatives of crops.

Kerstin Hoppenhaus has been working as a freelance director of documentaries, research films, and online projects since 2005. Before that, she studied biology in Mainz, Tübingen, Lyon, and Jena in addition to studying directing at the Film Academy Baden-Württemberg. Ms. Hoppenhaus has been awarded numerous prizes for her projects, including the Peter Hans Hofschneider Research Prize for Scientific and Medical Journalism. The HITS jury of science journalists and scientists selected her from among candidates from six continents to be the "Journalist in Residence" for 2018.

What exactly comes to mind when Kerstin Hoppenhaus thinks of her time at HITS? "I'm still surprised at how quickly the six months went by," she says. Ms. Hoppenhaus came to the institute with the aim of better understanding the interplay between science and data and – if possible – to develop new media formats for covering science. "I've learned a lot about data: for example, about graphical processors and machine learning," she says, and "it has all finally begun to sink in." Ms. Hoppenhaus had particularly in-depth discussions with chemist Frauke Gräter and computer linguist Michael Strube, who have both been working on an interdisciplinary project that deals with the effect of language in life science publications and makes use of machine learning methods. During her stay, Kerstin Hoppenhaus gave a very well-attended internal, interactive seminar on the communication of complexity and uncertainty on the Internet and also gave a public lecture entitled "Is there life after television?" Moreover, Ms. Hoppenhaus used her stay to visit other institutes in Heidelberg, the KIT in Karlsruhe, and colleagues at the SWR in Baden-Baden. Furthermore, she developed some project ideas "on the side." For example, Ms. Hoppenhaus worked with Vincent Heuveline on a project sketch for a modular tutorial in the field of artificial intelligence. "I would also like to develop a series of interviews on 'error logs' – that is, on errors in data research," Ms. Hoppenhaus explains. She had already planned one project before her stay: the "Unken-Postille", a hyperlocal science magazine based in the Uckermark region in Northeastern Germany, where she lives, that she is currently developing together with local residents. "I have to go now," Kerstin Hoppenhaus says. Her ten minutes on the phone have come to an end. The woman sure does know a thing or two about timing.

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PORTRAIT