



10 years of HITS - a reason to celebrate

On 1 January 2020, HITS will celebrate its 10th anniversary. For this occasion, the Institute has organized several special events and activities, also including its complete history – or "HITStory": It all began in 1997 when Klaus Tschira and his foundation created the EML European Media Laboratory, the nucleus for HITS, which continues to be supported by the Klaus Tschira foundation.

The Open House event on 11 July 2020 will provide visitors a glimpse into data-driven science at HITS and will include hands-on stations, science slams, and more. There will also be a guided tour through the garden for the first time. Moreover, the Institute will organize several events in the city of Heidelberg: HITS scientists will give talks on their research fields and topics in German that are targeted toward the public at large. These talks will report on the advantages of artificial intelligence for scientific research, how useful computer simulations are, and how interdisciplinary research works – from molecular biology to astrophysics.

In an extra weblog on the portal "Scilogs," ten "top stories" will highlight the most prominent HITS research projects, which range from the most detailed computer simulation of the Universe (which became the visual of a special stamp issued by the German Postal Service) to the decoding of the Axolotl genome.

The basic research at HITS centers around methods and software aimed at helping us to acquire new knowledge from a constantly growing volume of data. This goal is in line with HITS' motto: Think beyond the limits!



"HITS will be a very multidisciplinary institute." (Klaus Tschira at the opening event for HITS, March 2010)





MBM group leader **Prof. Frauke Gräter** has been appointed Fellow of the Max Planck Schools, a joint initiative between German universities and German research organizations. Through her position, she will mentor students, give a series of lectures, and organize workshops at the Max Planck School "Matter to Life."

Kai Polsterer, Vice President of the International Astroinformatics Association

AlN group leader **Dr. Kai Polsterer** has been appointed Vice President of the recently inaugurated "International Astroinformatics Association" (IAIA). The organization aims to foster the development of the global astroinformatics community, increase the professional recognition of the field, and provide a forum for the exchange of ideas and tools.

Gesa Schönberger, member of the BMBF "Strategic Foresight" initiative

HITS managing director **Dr. Gesa Schönberger** is a member of the "Zukunftskreis" (future working group) established by the Federal Ministry of Education and Research (BMBF). The working group is part of the recently launched "Foresight Process" that will study the development of societal values and the technological and social changes that society will face in the coming decade.

New employees and visiting scientists

- CCC: Anna Piras, doctoral student; Dr. Christopher Ehlert, postdoc
- DMQ: Philipp Lösel, research associate
- GRG: Johannes Horn, doctoral student; Marta Magnani, visiting scientist
- **MBM:** Matthias Brosz, doctoral student; Dr. Camilo Aponte-Santamaría, visiting scientist (Universidad de los Andes, Colombia) **MCM:** Madhura De, visiting scientist (DKFZ, Heidelberg); Abraham Muniz Chicharro, doctoral student;
 - Manuel Glaser, research associate
- PSO: Dr. Johann Higl, postdoc; Javier Morán Fraile, doctoral student

HITS groups (12/2019): 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).

HITSTERS

The irresistible pull – When massive stars collide

All neutron stars are magnetic, but some are more magnetic than others. These more highly magnetic, so-called



magnetars are the strongest magnets in the Universe. Their exceptionally large magnetic field is most probably due to the fact that they form in the supernovae of already highly magnetized stars. But how do these massive stars acquire their large magnetic field? Astrophysicists from Germany and the UK may now have solved this more than 70-year-old mystery of the origin of strong magnetic fields in massive stars. With the help of large computer simulations, they developed a model that demonstrates that these strong magnetic fields can be formed in stellar mergers. The results were published in October 2019 in the scientific journal Nature with a front-page picture.

"About 10% of more massive stars have a strong, large-scale surface magnetic field whose origins have eluded us since their discovery in 1947," says **Dr. Fabian Schneider** from Heidelberg University, first author of the study. It is these stars that astronomers believe form highly magnetic neutron stars when they explode in supernovae. This suggestion was confirmed by simulations on the HITS computing clusters using the AREPO code. The scientists showed that a strong magnetic field is indeed produced thanks to the strong shear and large turbulence present in the merger of two stars. Stellar mergers occur frequently, and about 10% of all massive stars in the Milky Way are thought to be the products of stellar mergers – a good match with the occurrence rate of magnetic stars.

Tau Scorpii (τ Sco) is one such star that was investigated. The researchers suggested that this star may also have obtained its strong magnetic field in the merger process.

At the end of its life, τ Sco will explode in a supernova when its core collapses and will most probably leave behind a highly magnetized neutron star. "These magnetars are thought to have the strongest magnetic fields in the Universe – one hundred million times stronger than the strongest magnetic field ever produced by humans," says **Prof. Friedrich Röpke**, leader of the Physics of Stellar Objects group at HITS. "Our simulations demonstrate that the generated magnetic field could be sufficient to explain the exceptionally strong magnetic fields believed to exist in magnetars," Dr. Schneider concludes.

Fabian R. N. Schneider. Sebastian T. Ohlmann. Philipp Podsiadlowski. Friedrich K. Röpke, Steven A. Balbus, Rüdiger Pakmor & Volker Springel: Stellar mergers as the origin of magnetic massive stars. Nature, volume 574, pages 211–214 (2019).



Ganna (Anya) Gryn'ova: "We want to get to the very core of the matter."

Her office window overlooks the HITS garden, its trees dazzling in their autumnal colors. "This is a place where people think," Dr. Ganna (Anya) Gryn'ova says. "And that's why I like it here." Since April 2019, the 32-year-old chemist has headed the new junior group Computational Carbon Chemistry (CCC) at HITS. Additionally, she is affiliated with Heidelberg University's Interdisciplinary Center for Scientific Computing (IWR) as a junior group leader.

The CCC group uses state-of-the-art computational chemistry to explore and exploit organic materials, such as graphene. "These systems offer many advantages over conventional inorganic counterparts, like being biocompatible, extremely variable in structure, and mechanically flexible," Dr. Gryn'ova explains.

Although the group addresses practical topics such as environmental chemistry, it does not aim to build devices. As theoreticians, the group's members instead focus on elucidating fundamental chemical insights and developing new material design concepts. "We want to get to the very core of the matter," Ganna Gryn'ova says.

Her motivation for basic research stems from her time at school. "I often had the feeling that science teachers didn't convey the whole picture. But I wanted to get to the bottom of things." Later, Ganna Gryn'ova studied chemistry at the Oles Honchar Dnipro National University, Ukraine, before pursuing a Ph.D. in computational chemistry at the Australian National University, Canberra. She completed her postdoc at École polytechnique fédérale de Lausanne, Switzerland, and was awarded the Marie Skłodowska-Curie Actions Individual Fellowship by the European Commission in 2016.

But why study graphene? "The chemistry of graphene-based materials lies at the intersection of what I know, what I want to know, and what others want to know," she says. Dr. Gryn'ova believes that modern computational chemistry tools might help us to better understand the fascinating features of this 'amazing material.' As she states, "We want to provide a link between trial-and-error discovery and rational design."

After eight months at HITS, Dr. Gryn'ova is even more impressed with the Institute. "We have something special here that not many places have and that must be cherished and preserved." Dr. Gryn'ova calls this "something special", the "spirit of HITS," which is characterized by the charm of a small and friendly institute with a dedicated working attitude. She enjoys the calm of her office with its inspiring view – "I imagine that's what it was like in ancient Greece," she smiles, "when people simply thought."

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