

## ERC Advanced Grant for HITS group leader

Mathematician **Anna Wienhard**, head of the “Groups and Geometry” group at HITS, has been awarded an ERC Advanced Grant – a prestigious grant for outstanding scientists



from the European Research Council (ERC). For her project on symmetries in mathematics, Wienhard will receive ca. two million euros over a period of five years. Wienhard is also a professor at the Mathematical Institute of Heidelberg University, the host institution for the ERC Grant.

Anna Wienhard has also received an ERC Consolidator Grant in 2014 for her work on symmetries and deformation spaces of geometric structures. The present project, “PosLieRep – Positivity in Lie Groups and Representation Varieties,” builds on the previous project and focuses on Lie groups, which play a central role in many fields of mathematics and are an important tool in theoretical physics.

“This is a great success and a clear sign of our close cooperation with Heidelberg University,” HITS Managing Director **Gesa Schönberger** stated. At present, a total of four ERC grantees work at HITS.

Since 2012, Anna Wienhard has been professor at the Mathematical Institute of Heidelberg University. She heads the Differential Geometry Research Group as well as the Geometry and Dynamics Research Station. Furthermore, she is co-spokesperson of the STRUCTURES Cluster of Excellence and a member of the Interdisciplinary Center for Scientific Computing.

Since 2015, Wienhard has also been leader of the “Groups and Geometry” group at HITS. Since October 2020, she has been Scientific Chairperson of the Heidelberg Laureate Forum Foundation, which organizes the annual Heidelberg Laureate Forum (HLF), a networking conference at which 200 outstanding young researchers in mathematics and computer science interact with recipients of the most-renowned prizes in the fields.



### Via Data

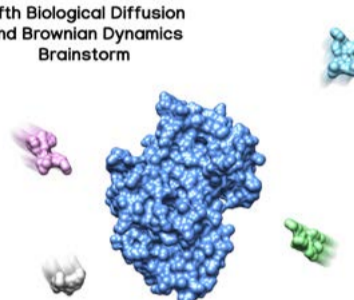
The HITS blog can be found on the “Scilogs” portal at <https://scilogs.spektrum.de/via-data/>.

## HITS

### BDBDB5: Online Workshop

On 24 and 25 March 2021, the 5th installment of the “Biological Diffusion and Brownian Dynamics Brainstorm”, in short: BDBDB5, took place online, with a new record of registered participants. MCM group members **Rebecca Wade**, **Stefan Richter**, **Ariane Nunes-Alves**, and **Abraham Muniz** organized the event, together with Rommie Amaro and Lane Votapka (both University of California San Diego). Since 2007, the BDBDB has been a forum for presentations and informal discussions about the current state of experimental and theoretical studies of biological diffusion, with a focus

### BDBDB5 Fifth Biological Diffusion and Brownian Dynamics Brainstorm



on the Brownian Dynamics method for simulating biological macromolecules. In a survey at the end of this year’s workshop, a majority of participants voted for the conference to be held more frequently.

### “Bioinformatics Advances”: Stamatakis associate editor

CME group leader **Alexandros Stamatakis** has been appointed as an associate editor for “Bioinformatics Advances”, an interdisciplinary journal on bioinformatics and computational biology. It covers bioinformatics methods, such as algorithms, statistics, databases and software as well as biological contributions for which the application of advanced computational methods is an essential factor. The major focus of the journal is on the molecular and cellular levels of biology.

### New employees and visiting scientists

**Administration:** Barbara Port, Scientific Manager  
**AIN:** Francisco Pozo Nunez, research associate  
**CCC:** Juliette Schleicher, master student  
**CME:** Dimitri Höhler, doctoral student; Julia Schmid, master student  
**DMQ:** Jonas Roller, doctoral student  
**GRG:** Fernando Camacho Cadena, doctoral student  
**MCM:** Giulia D’Arrigo, postdoc; Anna Mazurek, visiting scientist (medical university of Warsaw, Poland); Giulia Paiardi, postdoc; Jonathan Teuffel, master student

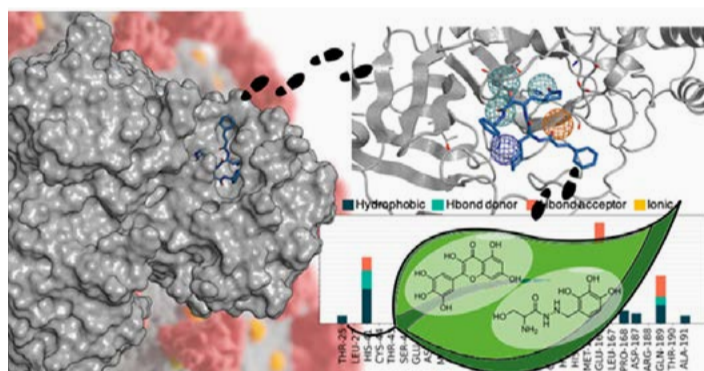
**MBM:** Jannik Buhr, visiting scientist (Heidelberg University); Christoph Karfusehr, master student; Aysecan Ünal, master student  
**NLP:** Wei Zhao, visiting scientist (TU Darmstadt, Germany)  
**SDBV:** Lukrécia Mertová, doctoral student  
**TOS:** Teresa Braun, master student

**HITS groups 06/2021:** 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

### Putting computing power together against SARS-CoV-2

The first vaccines authorized for use are raising hopes for an end to the pandemic. What is still missing, however, is an effective cure. Scientists



in the European consortia EXSCALATE4CORONAVIRUS (E4C) and the “Human Brain Project” (HBP) teamed up with other European research institutions to work on a novel computational approach, reported in a recent publication, by which they identified potent inhibitors of the SARS-CoV-2 main protease, a promising target for antiviral compounds.

In order to identify shapes of the binding site of the main protease that inhibitors might bind to, **Rebecca Wade** (MCM) and her group at HITS, along with colleagues at Forschungszentrum

Jülich (FZJ) and the Stockholm Royal Institute of Technology (KTH), investigated more than 30,000 possible spatial arrangements of the enzyme’s three-dimensional shape. The HITS researchers applied their TRAPP analysis tool to categorize these “individual snapshots” and

identify the best-fitting structures. These structures were then virtually screened by the colleagues at FZJ. “This way, we calculated which molecules could theoretically fit into all these possible conformations and were able to define a blueprint for high affinity compounds”, explains Giulia

Rossetti (FZJ). This research demonstrates the value of interdisciplinary trans-European networks and infrastructures, such as E4C and HBP, when it comes to pooling expertise and resources and developing new approaches to drug discovery. In further work, the researchers will make use of the HBP’s FENIX infrastructure.

Gossen J., et al: A Blueprint for High Affinity SARS-CoV-2 Mpro Inhibitors from Activity-Based Compound Library Screening Guided by Analysis of Protein Dynamics. ACS Pharmacology & Translational Science Article ASAP DOI: 10.1021/acspstsci.0c00215

### The good, the bad, and the spaghetti code: Software put to the test

Digital tools are essential in science, particularly when large amounts of research data accumulate and have to be processed quickly. However, the development and maintenance of scientific software are often influenced by financial uncertainty and time pressure, which can lead to badly written code. In order to evaluate the software quality automatically, **Alexandros Stamatakis** and **Dimitri Höhler** (CME), together with colleagues from the Karlsruhe Institute of Technology (KIT), have designed the “SoftWipe” tool. “It offers a fast, reliable and cost-effective solution. In addition, the researchers ranked 48 tools from various research areas by evaluating how coding standards were adhered to. They found substantial differences in software quality. The authors therefore recommend that tools like “SoftWipe” should be used as standard in the selection and assessment process for scientific software.

Zapletal, A., Höhler, D., Sinz, C. et al.: The SoftWipe tool and benchmark for assessing coding standards adherence of scientific software. Sci Rep 11, 10015 (2021). <https://doi.org/10.1038/s41598-021-89495-8>

## Research

### Behind the Science: Heidelberg University



Last year, teams were introduced that work “behind the scenes” to make life for the researchers at HITS so much better in one way or another. Now, it is time to shed light on the board that makes the existence of the Institute

possible through its work “in the background”: the HITS shareholders. In this issue, Heidelberg University takes center stage, represented by Vice-Rector for Research **Jörg Pross**.

### Professor Pross, when did Heidelberg University become a HITS shareholder, and how did that come about?

Heidelberg University has been a shareholder since November 2014, with a share of 15 percent. However, our collaboration with the precursor institute to HITS – EML Research gGmbH – dates back to 2007, when a first agreement was reached. The joint appointment of astrophysicist Volker Springel in 2009/2010

was an important step. Since then, the partnership has continued steadily, and as of today, HITS and Heidelberg University are linked through four endowed professorships and numerous other activities.

### What is the University’s interest in being formally associated with HITS as a shareholder?

HITS contributes significantly to making Heidelberg even more visible and attractive as a hub for science. Joint appointments are an excellent tool for convincing top scientists to come to Heidelberg in the increasingly fierce competition for the brightest minds. The resulting synergies have been extremely beneficial for both sides.

### What do you think are the benefits of this association for HITS?

In general, HITS benefits from the charisma of Heidelberg as a hub for science and in turn contributes to this charisma – a self-reinforcing process that benefits everyone involved. In concrete terms, this close cooperation gives HITS researchers access to the many facets of the University’s research-supporting infrastructure, such as the offerings of the graduate schools. Many HITS group leaders are also professors at the University. Through their involvement in university teaching, these group

leaders have direct contact with students, many of whom they are able to inspire to write a doctoral thesis, which is completed by a doctoral degree. The doctorate, which can as a rule only be awarded by a university, is then structured and granted by Ruperto Carola.

HITS junior group leaders can also complete post-doctoral research through the University and thereby decisively shape their academic careers.

### What makes HITS so exciting to you?

I am enormously impressed by the science-driven atmosphere at HITS – for me, that is academic freedom in the best sense. I have the greatest respect for the founder, Klaus Tschira, and his vision. The ability to conduct research with an absolute minimum of administrative complications is both a privilege and a responsibility. It makes HITS a unique project.

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## Behind the Science



## The Charts