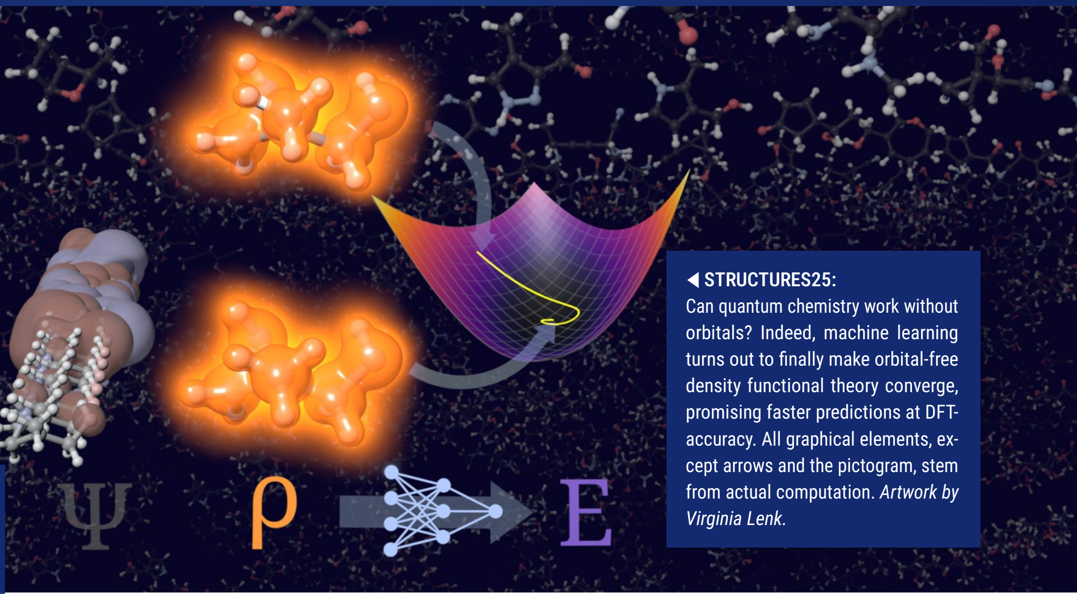
STRUCTURES | NEWS

STRUCTURES CLUSTER OF EXCELLENCE

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386



◀ **STRUCTURES25:** Can quantum chemistry work without orbitals? Indeed, machine learning turns out to finally make orbital-free density functional theory converge, promising faster predictions at DFT-accuracy. All graphical elements, except arrows and the pictogram, stem from actual computation. *Artwork by Virginia Lenk*.

October 2025

Contents

Upcoming

- **STRUCTURES Jour Fixe**: TBA
- **Rhind Seminar:** Nov 3, 10, 17, …
- **Application for Les Houches Summer School 2026:** Deadline 1st december

Further details can be found at: https://structures.uni-heidelberg.de

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RESEARCH

New Machine Learning Model Advances Decades-Old Quantum Chemistry Puzzle

Researchers at Heidelberg University have made a significant advance in computational quantum chemistry with the development of STRUCTURES25, a new orbital-free density functional theory (OF-DFT) method powered by machine learning.

In the 1960s, physicists Hohenberg and Kohn made a landmark discovery: the ground-state energy of a molecule or material is completely determined by its electron density — a function describing where electrons are most likely to be found. In principle, this meant that the complex, many-body equations of quantum mechanics could be replaced with a simpler task: finding the energy density functional in terms of this density and minimizing it.

For decades, however, sufficiently good approximations for the *universal kinetic energy density functional* have remained unknown, requiring the use of *Kohn–Sham density functional theory (KS-DFT)* instead – where auxiliary wave functions or *orbitals* were reintroduced. While highly successful in practice, the computational cost of KS-DFT can be prohibitive for larger systems, prompting renewed interest in orbital-free density functional theory.

Within our cluster, the Hamprecht and Dreuw groups, combining their expertise in machine learning and quantum chemistry, have been developing a new method to learn it directly. Their current model, *STRUCTURES25*, achieves chemical accuracy in energy predictions and successfully converges to physically meaningful electron densities for small organic molecules, a long-sought goal that could revolutionize the efficiency of calculations for huge molecular systems. Augmenting the training data with densities obtained from perturbed potentials proved key to these results.

With these advances, the team has brought Hohenberg's and Kohn's original vision a big step closer to reality — and opened the door to fast, accurate quantum-level modelling of systems far beyond the reach of today's most widely used methods.

Original Publication:

R. Remme, T. Kaczun, T. Ebert, C. A. Gehrig, D. Geng, G. Gerhartz, M. K. Ickler, M. V. Klockow, P. Lippmann, J. S. Schmidt, S. Wagner, A. Dreuw, and F. A. Hamprecht, Journal of the American Chemical Society, DOI: 10.1021/jacs.5c06219.

RESEARCH

Gravitational Turbulence Explains Universal Scaling Law in Cold-Dark-Matter Cosmology

In our current understanding of structure formation, halos of cold dark matter grew from tiny fluctuations via gravitational collapse. Smaller clumps formed first and merged into bigger ones, creating potential wells for stars and galaxies to form.

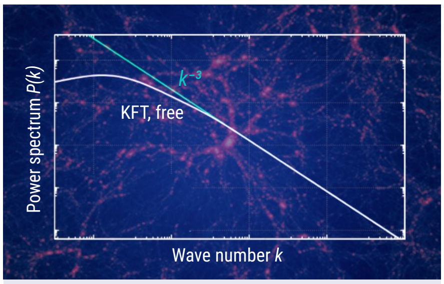
Cosmological simulations show that the dark matter power spectrum – a measure of how much structure exists at different scales – converges at high resolution towards a k^{-3} power law with the wave number k on small scales, consistent with observations. Despite its simplicity, this power law has lacked a theoretical foundation, leaving researchers reliant on costly N-body simulations to test different assumptions on dark matter, cosmology or initial conditions.

In a new study, researchers from STRUCTURES, Oxford and Princeton showed that cold dark matter in d spatial dimensions universally develops a k^{-d} asymptotic scaling. They propose a theoretical explanation for this scaling based on two complementary derivations: from *Kinetic Field Theory (KFT)* – an analytic framework for structure formation developed in Heidelberg – and from the evolution of the phase-space distribution under the *Vlasov equation*. According to the new study, gravitational collapse drives a turbulent cascade in which dark matter streams fold and twist in phase space, with the universal scaling emerging as the only stable outcome.

This discovery builds on earlier work. In 2022, the STRUCTURES team around Sara Konrad and Matthias Bartelmann had shown that within the so-called *Zel'dovich approximation*, a k^{-d} tail forms independently of the cosmological model or the initial matter distribution.

The new study generalizes this result beyond approximations and provides a physical mechanism. These insights are important for testing models of gravity and structure formation, understanding the nature of dark matter, as well as for the theory of gravitationally driven turbulence. The results may also help explain the universal density profiles of dark matter halos seen in simulations, a long-standing cosmological enigma.

Simulation of twists and rotations in the phase-space distribution of cold streams in one spatial dimension. *From Ginat et al. 2025 (CC-BY 4.0), colours modified.*



Matter power spectrum at early times predicted by KFT. *Adapted from Konrad & Bartelmann 2022. Background image: Visualization of dark matter filaments (Credit: Illustris Collaboration).*

Related Publications:

1. Ginat, Y. B., Nastac, ..., Konrad, S., Bartelmann, M. 2025, *Phys. Rev. D*, 112, 6, 063501. doi:10.1103/ychs-2d5p.
2. Konrad, S., Ginat, Y. B., & Bartelmann, M. 2022, *MNRAS*, 515, 4, 5823. doi:10.1093/mnras/stac2064.
3. Konrad, S. & Bartelmann, M. 2022, MNRAS, 515, 2, 2578. doi:10.1093/mnras/stac1795.

STRUCTURES EVENTS

Schöntal Discussion Workshop 2025: Inverse Problems

For four days in August, sixteen students and two professors gathered at the beautiful Schöntal Abbey to study and discuss about the topic of *Inverse Problems*. Participants were organized in four groups, each of which carefully prepared subtopics, and presented them during the workshop, leading to in-depth discussions. The Schöntal workshop was thus a lively and enriching experience!

The annual workshop, funded by STRUCTURES' *Young Researchers Convent (YRC)*, brings together early-career researchers from different areas of STRUCTURES to engage in discussion over topics that go beyond the standard curriculum of a lecture. This year's workshop, marking its ninth edition, was organized by Rebecca Maria Kuntz, Carlos Pastor Marcos, Hannes Heisler, and Sander Hummerich.

YOUNG RESEARCHERS CONVENT

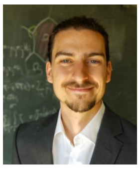
Any student (BSc, MSc, PhD) or postdoc whose work fits into the concept of STRUCTURES can apply for YRC membership. If your supervisor is a STRUCTURES member *or* your work is funded by STRUCTURES, you are *directly eligible* for membership. For more details, *visit https://structures.uni-heidelberg.de/YRC.php.*

STRUCTURES COMMUNITY

STRUCTURES Welcomes New Members

STRUCTURES warmly welcomes four new members, elected by last July's General Assembly: Claudia Strauch, Tim Laux, Julian Schmitt, and external member Giacomo Gori. With their expertise spanning from mathematical foundations to cutting-edge experimental research, they will further strengthen our interdisciplinary research community. We wish all our new colleagues a good start and look forward to many exciting joint projects and exchanges!

Claudia Strauch
Professor for Mathematics
Statistics of Stochastic Processes



Tim Laux
Professor for Mathematics
Applied Geometric Analysis

Julian Schmitt
Professor for Experimental Physics
Optical Quantum Systems

Giacomo Gori
Postdoc (external member at CNR-INO)
Condensed Matter Theory

EQUAL OPPORTUNITIES

YAM: Building Bridges Across Continents – Interview with Mina Chavelle Tchoua Tchoua

Since 2023, STRUCTURES has been a partner of the *Young African Mathematicians (YAM)* programme – a joint cooperation between four German clusters of excellence and the five centres of the *African Institute for Mathematical Science (AIMS)*. The initiative enables outstanding AIMS Master graduates to spend an academic year at a renowned mathematical institution in Germany, conducting independent research and immersing themselves in a dynamic research environment.

More than training scientific competence, the idea of YAM is to foster collaboration and to build lasting academic bridges. Fellows are encouraged to explore new ideas, connect with peers and mentors, and expand their international networks.

In our newsletter we regularly introduce YAM fellows and their stories. For this edition, we have interviewed 2024/25's fellow Mina Chavelle Tchoua Tchoua, who has completed her one-year fellowship in Heidelberg and will attend a PhD position in Orléans. In her research, she developed a *Bayesian Operator Framework* for polynomial model inference, in order to efficiently solve inverse problems in the context of *partial differential equations (PDEs)*. The framework enables learning the mapping from coefficient fields to solution fields.

Interview with Mina C. Tchoua Tchoua:

What motivated you to apply for the YAM programme?

I was motivated to apply for the YAM programme because I wanted to explore mathematical ideas beyond my academic background and connect with researchers from different disciplines while experiencing the vibrant academic environment in Heidelberg. The opportunity to collaborate with Prof. Jakob Zech was particularly appealing.

How was your time at STRUCTURES, and what did you take away from it?

My time at STRUCTURES was incredibly enriching both academically and personally. I learned a lot from discussions with researchers and students, and it helped me gain confidence in pursuing independent research. The supportive environment made it a truly memorable experience.

What excites you about mathematics?

I love how mathematics allows us to describe complex phenomena with elegant simplicity. It's a universal language that connects ideas across different fields.

How has the YAM fellowship influenced your academic path?

The fellowship helped me strengthen my research skills and clarify my long-term goals. It played an important role in my decision to pursue a PhD and continue exploring mathematical models in depth.

Mina Chavelle Tchoua Tchoua, YAM fellow 2024/25.

Group picture from the 2025 YAM network meeting in Heidelberg, hosted by STRUCTURES.

What advice would you give to future YAM fellows or early-career scientists considering similar opportunities?

Stay curious and open-minded. Make the most of the international environment, talk to people, share your ideas, and don't hesitate to explore new directions. STRUCTURES has an incredible network of researchers who are genuinely happy to share their knowledge. Also, take time to explore Heidelberg and connect with other fellows.

STRUCTURES EVENTS

ENUMATH Conference Brings Together Over 600 Numerical Mathematicians

From September 1–5, 2025, Heidelberg University hosted the *European Conference on Numerical Mathematics and Advanced Applications (ENUMATH)*, supported by the STRUCTURES Cluster of Excellence.

More than 750 researchers from over 30 countries gathered for plenary talks, minisymposia, and poster sessions covering topics from discretization and multiscale modelling to uncertainty quantification, optimization, and scientific machine learning.

Chaired by STRUCTURES member Robert Scheichl and organized with colleagues from STRUCTURES, the *Interdisciplinary Center for Scientific Computing (IWR)*, and the *Institute for Mathematics (IMa)* – the conference fostered international exchange and collaboration in these thriving fields.

Photo credits: Robert Scheichl, Peter Bastian, Anima Kujur

ANNOUNCEMENTS

Les Houches Summer School 2026: Quantum Theory On All Scales

We are pleased to announce the 2026 Les Houches Summer School on *Quantum Theory on All Scales*, taking place August 03-28, 2026 in the idyllic location of Les Houches in the French Alps. The school, which is supported by STRUCTURES, aims to highlight recent significant progress on the mathematical analysis of complex quantum systems, and to discuss interesting open questions for the future. Six lectures, along with numerous short courses and talks, will focus on interacting and correlated systems, as well as random systems – with methods drawn from analysis and probability to algebra and topology.

The last Les Houches school with this focus took place in 2010 under the title *Quantum theory from small to large scales*.

It brought together many of the best doctoral students and postdoctoral researchers in the field and from all over the world and gave them a perspective beyond their specific thesis and research work. It further led to lasting research connections, friendships and a sense of community. Many of those that attended the 2010 school as PhD students and postdoctoral fellows have since been appointed as faculty at major research universities.

Cécile DeWitt-Morette
Founder of Les Houches School of Physics (1922 - 2017)

Les Houches School of Physics is proud to have been welcoming physicists from around the world since 1951. Founded by French physicist Cécile DeWitt-Morette, the school has trained generations of early-career researchers, some of whom have since won Nobel prizes.

Application is open until December 1st, 2025. Please find more information at:

Website: Les Houches Summer School "Quantum Theory on All Scales"
https://structures.uni-heidelberg.de/events/les_houches_2026/

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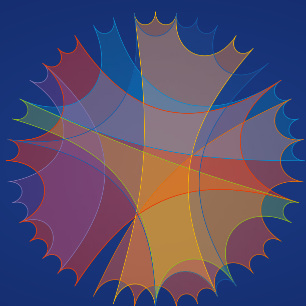

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