Leibniz Fast Calulation Competition
Call for participants

International Competition on Accelerating Diffusion Calculation for Molecular Dynamic Simulation

Developing advanced methodologies including algorithm optimization, potential function creation, etc. to accelerate molecular dynamic simulation (MD) tailored for diffusion phenomenon at the interface.

About the Competition

This global event welcomes researchers, scientists, and computational enthusiasts to push the boundaries of current MD simulation capabilities. The competition aims to foster innovation and collaboration and seeks to identify and promote new methods and technologies that can significantly enhance the speed and accuracy of MD simulations, particularly focusing on diffusion at interfaces. The international competition encourages a collaborative spirit via idea and data sharing. The FAIR principles ensure that the data is accessible, reusable, and can be integrated into future research, enhancing the overall impact of advancing MD simulations. All the contributions will be published in the Open Research Knowledge Graph (orkg.org).

Starting point

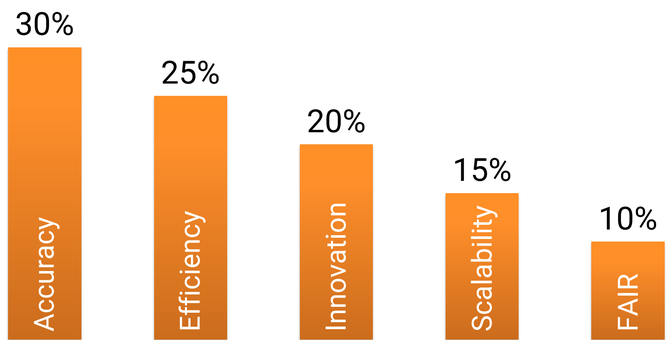
- **Case study template**
  Lammps infile of a diffusion study between copper (Cu) and aluminum (Al) at oxygen-free atmosphere using the embedded atom method potential
- **Documentation**
  Usage of the infile
  Installation of LAMMPS and Ovito
  Access to computational resources
- **Data management guideline**
  Instructions on how to manage data in compliance with FAIR principle
- **Submission guideline**
  Instructions on the submitted files, format, contents, size, etc.

Outputs

- **Diffusion coefficient**
  Diffusion coefficient value
  Calculation method
- **Documentation**
  Workflow (following FAIR principles)
  Methodology description, e.g. optimized algorithm or potential function or simulation setup, etc.
- **Results**
  Log files, image sequences, animations, post-processing files/codes
- **Simulation performance**
  Information of the size, time, and speed of simulations using CPUs/GPUs

Evaluation

Solutions will be assessed based on accuracy, computational speed, scalability and innovation for developing the fastest and most accurate method for simulating the diffusion between Al and Cu at low temperatures. FAIR principles ensure that the data is findable, accessible, interoperable and reusable.



Scientific Committee

Nina Merkert (TU Clausthal, Germany)
Shan Lyu (TU Clausthal, Germany)
Hoàng-Thiên Luu (TU Clausthal, Germany)
Iryna Mozgova (Universität Paderborn, Germany)
Andreas Schultz (Universität Paderborn, Germany)
Oliver Koepler (TIB Hannover, Germany)

Key dates

Registration: until September 15th, 2025

Deadline for Submissions: January 20th, 2026

Evaluation: January 21st, 2026 - March 12th, 2026

Prizes*

1st Prize
- Certificate of Excellence
- A 3-month stay as a visiting researcher at the SFB featuring a monthly expense allowance of 1300 € and a travel allowance.
- Coverage of a joint Open Access publication.

2nd Prize
- Certificate of Excellence
- A 1-month stay as a visiting researcher at the SFB featuring a monthly expense allowance of 1300 € and a travel allowance.

3rd Prize
- Certificate of Excellence

*Terms and conditions apply. For details, please visit https://www.sfb1368.uni-hannover.de/en/competition

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Organized by the Collaborative Research Center 1368 “Oxygen-free Production”

Register now under: www.sfb1368.uni-hannover.de

CRC 1368 Oxygen-free Production
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