

CELEST Member Short Profile



Wolfgang Wenzel

Wolfgang Wenzel, leads the department of multiscale modelling and materials design at the Institute of Nanotechnology at Karlsruhe Institute of Technology. He obtained his Ph.D. in Physics in 1989 at Ohio State University before moving first to Dortmund University and then to Karlsruhe University. His research interests are the development and application of multi-scale simulation methods to nanoscale structure formation and function. Further development of these methods, he is actively involved in the EU project BIG-MAP on batteries and the coordination of the joint lab for virtual materials design of the Helmholtz association.

Institute of Nanotechnology (INT)

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Research areas

His main research objectives are the development and application methods for multi-scale simulations of nanoscale materials and devices. The key goal of the method is the development of predictive scale-bridging methods for materials design and discovery via interlinking several different spaces and/or time scales to construct an accurate model and implemented it in workflows.

Lab equipment (at INT, campus north of KIT)

Hardware: High Performance Computing cluster with 512 cores and GPU with 32 cores
 Software: Molecular Dynamics Programs (GROMACS, LAMMPS, AMBER/AMBERTOOLS, NAMD, Coarse-Grained Model); Quantum Programs (TURBOMOLE, VASP, CP2K, MOPAC, Octopus, ORCA); Visualization Programs (VMD, Pymol, Ovito, Jmol, UCSF Chimera, VESTA, Molden, Avogadro, ase-gui); Wenzel developed Programs (SIMONA, SIMSTACK).

Wolfgang Wenzel @ INT

https://www.int.kit.edu/1632_wolfgang.wenzel.php

Link INT

<https://www.int.kit.edu/index.php>

Link lab equipment

<https://int-wenzel-wiki.int.kit.edu/>

Partners