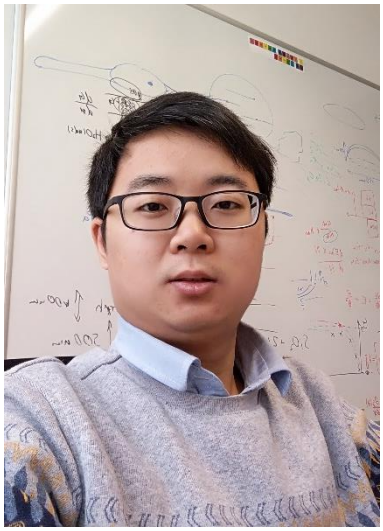
## Dr. Xiao Hu

Center for Microtechnologies, Technische Universität Chemnitz | Scientific employee



Dr. Xiao Hu studied microelectronics at Technische Universität Chemnitz, where he obtained a Ph.D. degree in 2017 under the supervision of Prof. Schulz and Prof. Geßner. His dissertation was devoted to the multiscale simulation of copper ALD. Since 2017 he has been a scientific employee at Center for Microtechnologies, Technische Universität Chemnitz. Currently, he serves as the principal investigator of a DFG project with focus on the rational design of selective thermal atomic layer etching processes. His research concentrates on the surface chemistry of thin film deposition and etching processes. He is also working on the development and application of atomic and molecular simulation methods.

### *"Atomistic simulations of atomic layer processes"*

March 25, 2021 | 13:50 – 14:10

With the rapid improvement of computer performance, atomistic simulations have become a powerful tool to understand and predict material properties. In the lecture, we will illustrate the use of atomistic simulations to investigate the chemical mechanisms of atomic layer processes, in particular ALD and thermal ALE. Different simulation methods, including density functional theory, molecular dynamics, and kinetic Monte Carlo simulations, will be introduced and discussed. The combination of these methods provides detailed information for atomic layer processes over a wide range of length and time scales. Based on examples of metal and metal oxide ALD, we will demonstrate how the ALD reactions can be predicted using atomistic simulations. Most of the predicted results are validated and directly compared with experimental data. Thermal ALE has emerged as a new technique for the isotropic etching of materials with atomic-scale precision. Here, we chose thermal $Al_2O_3$ ALE using HF and $Al(CH_3)_3$ as a case study. Based on a mechanistic understanding of ALE reactions, we will discuss the strategies for the design and screening of precursors.