Institut für GEOWISSENSCHAFTEN und GEOGRAPHIE
Martin-Luther-Universität Halle-Wittenberg

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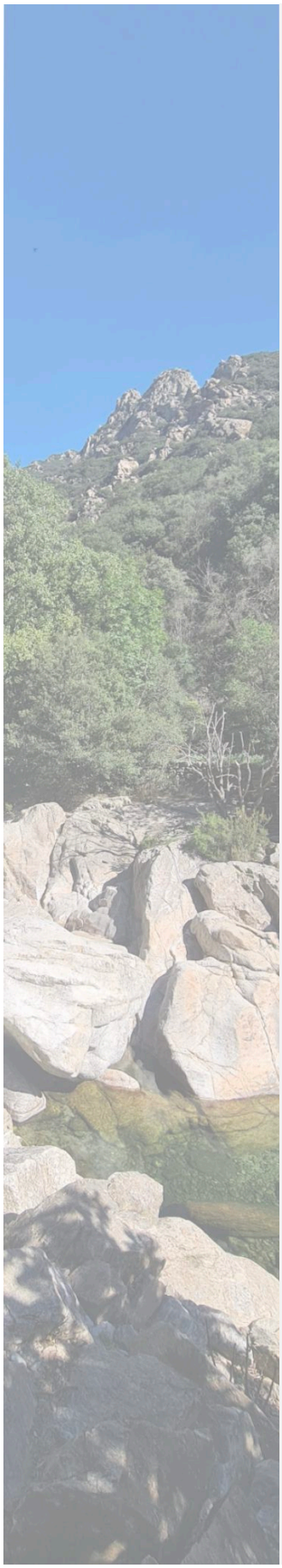
HALLE-WITTENBERG

Geowissenschaftliche Kolloquien WiSe 2025/2026



Mo 19.01.2026
17.15 Uhr

Herr PD Dr. Michael Fischer

Fachbereich Geowissenschaften der Universität Bremen,
Fachgebiet Kristallographie und Geomaterialforschung

Computational modelling of zeolites for environmental applications: From predictive simulations to fundamental understanding

PD. Dr. Michael Fischer

Zeolites are natural or synthetic tetrahedral framework materials exhibiting an intrinsic porosity. They are already used on an industrial scale in catalysis, ion exchange, and gas separation. Beyond established fields, zeolites have also been proposed (and, in some instances, employed) for various applications that are related to the prevention or remediation of environmental pollution. Potential uses in this area include the capture of carbon dioxide and other airborne pollutants, the removal of organic contaminants like pharmaceuticals and personal care products (PPCPs) from water, and the adsorption of environmentally harmful ions from water and soils. Although atomistic simulations cannot replace experiments under real-world conditions, they can make useful predictions and deliver additional insights that cannot be obtained experimentally. In this talk, I will present results from computational investigations at different levels of theory, which are aimed at potential environmental applications of zeolites that range from carbon dioxide capture to the removal of PPCPs from aqueous solution. Where possible, I will establish links between simulation results and experimental observations, as well as highlighting remaining challenges and future opportunities.