

VIRTUAL MATERIALS DESIGN

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Karlsruhe Institute of Technology, Karlsruhe, Germany Arguably, simulation has emerged as a third pillar of the scientific endeavor, complementing experiment and analytical theory. However, in many scientific fields, including materials science, the simulations are more often used to explain observations rather than a to predict the behavior of new materials. In order to increase the predictive role of simulations my group and others have teamed up to systematically develop methods for virtual materials design.

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