

# Materials simulation: from interpretation to prediction

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**Auditoire B02** Campus Kirchberg

Over the past two decades computational science has evolved into a paradigm-changing research approach. In this time, computer speed has increased nearly a million fold, while the new algorithms and numerical methodologies that have been developed facilitate more accurate simulations and more efficient data exploration. This progress has had a profound impact on materials research, advancing computation from a mere means to interpret experimental data to a tool for the design and discovery of novel materials. In this presentation I will give a brief historical overview and outlook with regards to the role of computation in science and engineering, and then present a few examples from our own research illustrating the use of materials simulation. These examples include the unveiling the nature of anomalous thermo-mechanical properties of network glasses, the prediction of new crystalline oxide phases, and a scheme for developing novel organic semiconductors for photovoltaic or solid state lighting applications based on rapid screening of candidate molecules using simulation.

*John Kieffer studied metallurgy and obtained a PhD in materials science from the University of Clausthal in 1985. He held research positions at Arizona State University, Purdue University and Saint-Gobain Recherche in Paris. From 1995 to 2001 he was assistant, then associate professor at the University of Illinois at Urbana-Champaign before joining the University of Michigan where he became full professor in 2005. He is a Fellow of the American Ceramic Society and in 2007 he received the Materials Science and Engineering Outstanding Achievement Award. He has authored more than 80 papers in peer-reviewed journals.*

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**Dan Zachary** Embry-Riddle Aeronautical University Luxembourg Campus

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