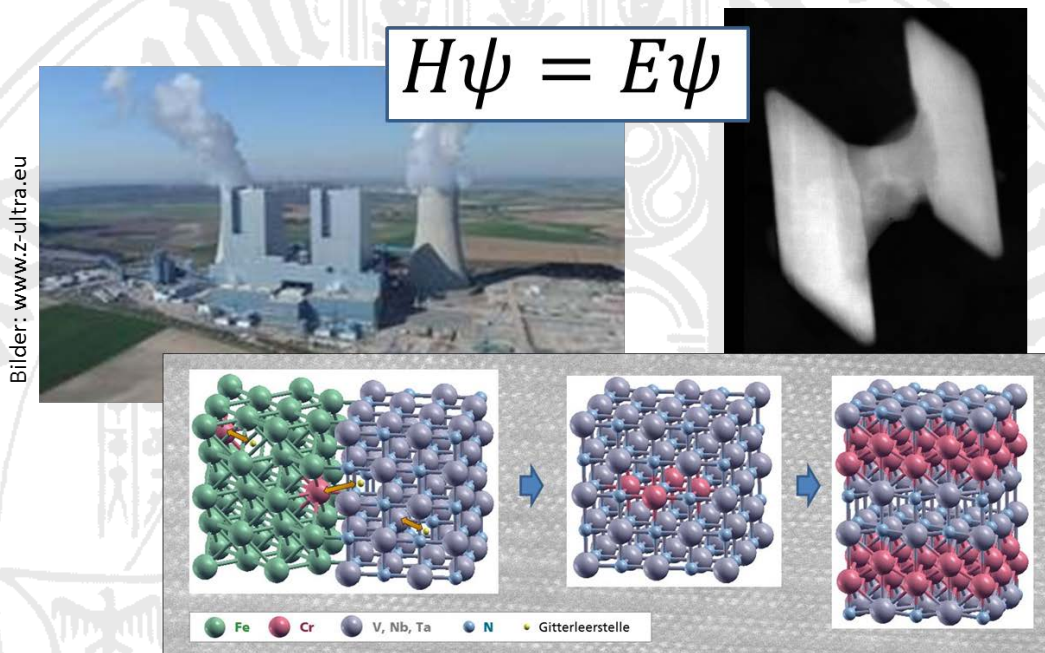


PHYSIKALISCHES KOLLOQUIUM

AM 9. JULI 2018 UM 17 UHR C.T.

IM GROßEN HÖRSAAL



MATERIALS DESIGN INSPIRED BY THEORETICAL PHYSICS: FROM SCHRÖDINGER'S EQUATION TO POWER PLANTS

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How can atomistic modelling and simulation assist the design and discovery of new functional materials? Can we really make more efficient and longer lasting materials with targeted physical properties and functions, consuming fewer resources, by solving the Schrödinger equation? And is this a task for a practical engineer or a theoretical physicist? In my talk I will report on a development of a new high-temperature corrosion-resistant steel to illustrate, how computer simulations based on density functional theory (DFT) are used to resolve the correlations between the physical and mechanical properties of a material with its atomic and electronic structures. We investigate the essential precipitation formation process using theoretical and computational methods based on solid-state physics and materials mechanics. Results on thermodynamic stability, atom diffusion, and phase transformation are the pieces of the puzzle to be joined for an understanding of the underlying mechanisms and relationships. Constructing this theoretical model enables the optimization of the new steel and supports experimental efforts to control its mechanical properties through appropriate microstructural engineering.