



Einladung zum Wilhelm-Ostwald-Institutskolloquium

Am Montag, dem 07.10.2019, 16:15 Uhr, spricht

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zum Thema:

Theoretical approaches in nanocatalysis and materials design

Abstract

Development of effective and environment friendly catalysts for energy related applications is an emerging task. In this presentation we will show that novel catalytic materials can be rationally designed from the scratch using theoretical approach and computer modelling followed by experimental verification. Instead of investigation of the well-known catalytic materials based on the precious metals, like Pt, Pd, Ru, etc. we have found the way how to functionalize abundant catalytically inactive or even completely inert nanomaterials and control their catalytic properties via support design and morphology. Thus, a novel class of electrocatalysts for oxygen reduction reaction (ORR) and hydrogen evolution reaction (HER) based on the inert and insulating two-dimensional hexagonal boron nitride (h-BN) has been predicted. Several examples of catalytic processes on free and supported atomic clusters, 2D structures and their heterojunctions with the support will be considered.