MM 9: Non-equilibrium Phenomena in Materials Induced by Electrical and Magnetic Fields 2

Material modification

Time: Monday 17:15–18:30 Location: H45

Topical Talk MM 9.1 Mon 17:15 H45

Design of corrosion-free and highly active electrocatalysts and photocatalysts via combinations of ab initio calculations and electrodynamics — •Heechae Choi — Institute of Inorganic Chemistry, University of Cologne, Greinstr. 6, 50939, Cologne, Germany

Long enough lifetime of a catalyst is a very important, and frequently overlooked issue in catalyst design and development. For catalytic materials used in extreme conditions, corrosion resistance is the key factor to determine the lifetime and the steady performances over time. However, the theoretical design principle for the corrosion resistance of catalytic materials is lacking compared to the performance descriptor, which can give accurate predictions of catalytic activities of metallic materials. Recently, using the combinations of ab initio calculations and electrodynamics model, we proposed a new theoretical scheme to improve the catalytic activity and corrosion resistivity. Under the hypothesis that the resistance of corrosion is a function of adsorption energy of corrosive ions in aqueous phases, we attempted to install built-in electric fields on heterogeneous catalyst surfaces. As the results, the performances of TiO2 photoanode, Co/graphene Zn-air battery, and the water splitting by metal/carbon hetereojunctions were highly improved. In this talk, I will introduce the procedures of such materials design theory developments and the experimental verifications.

MM 9.2 Mon 17:45 H45

Understanding DC-induced abnormal grain growth in FeC-thin films — •Thomas Brede, Michel Kuhfuss, Reiner Kirchheim, and Cynthia Volkert — Institut für Materialphysik, Universität Göttingen, Deutschland

The field of processing materials with magnetic or electric fields and currents in steadily growing, since it opens the door to more efficient ways of material treatment and former not achievable material modifications. In this scope, it was shown recently, that high DC electric current densities up to 4 MA/cm^2 can be used at elevated temperatures of 550°C to produce elongated ferrite grains with high aspect ratios in an otherwise nanocrystalline iron-carbon thin film. To understand the underlying mechanism we will present experiments in a wide range of process parameters. The samples were characterized by SEM and EBSD in different stages of the experiment. The results shown allow a detailed description of the underlying mechanism of the evolution of the abnormal grown structures. In addition they reveal a threshold linked to the electromigration-induced C-flux, below which no changes occur. A purely kinetic model will be presented to describe the observed behaviour and allow the prediction of similar effects at different process parameters and material systems.

MM 9.3 Mon 18:00 H45

Cavity induced and influenced phases of matter — •Christian J. Eckhardt[1,2], Giacomo Passetti[2], Marios Michael[1], Frank Schlawin[1], Dante M. Kennes[2,1], and Michael A. Sentef[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]RWTH Aachen University, Aachen, Germany

An optical cavity may be used to influence or induce phases of matter. We discuss how a charge-density wave phase in a 1-dimensional chain of spinless fermions is enhanced through the coupling to the quantized photon field. At the critical point between the Luttinger liquid and the charge-density wave, we find strong light-matter entanglement. Additionally, we ask in what ways photons can be used as pairing glue for superconductivity (SC). We show that a fingerprint feature of such cavity-induced SC is the pickup of a k-dependence of the gap in the electronic spectrum on the Fermi-surface.

MM 9.4 Mon 18:15 H45

Floquet engineering the band structure of materials with optimal control theory — •Alberto Castro[1,2], Umberto de Giovannini[3,4], Shunsuke Sato[5,4], Hannes Hübener[4], and Angel Rubio[4,6] — [1]ARAID Foundation, Zaragoza (Spain) — [2]Institute for Biocomputation and Physics of Complex Systems, University of Zaragoza, Spain — [3]Universitá degli Studi di Palermo, Dipartimento di Fisica e Chimica - Emilio Segrè, Palermo, Italy — [4]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [5]Center for Computational Sciences, University of Tsukuba, Tsukuba , Japan — [6]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, New York NY

We demonstrate that the electronic structure of a material can be deformed into Floquet pseudo-bands with tailored shapes. We achieve this goal with a novel combination of quantum optimal control theory and Floquet engineering. We illustrate this framework utilizing a tight-binding description of graphene. We show several examples focusing on the region around the K (Dirac) point of the Brillouin zone: creation of a gap with opposing flat valence and conduction bands, creation of a gap with opposing concave symmetric valence and conduction bands, or closure of the gap when departing from a modified graphene model with a non-zero gap. We employ time periodic drives with several frequency components and polarizations, in contrast to the usual monochromatic fields, and use control theory to find the optimal amplitudes of each component that optimize the shape of the bands as desired.