MA 45: Focus: Disorder Engineering as a Tool for Material Science

Organized by S. Chadov (MPI-CPfS Dresden) and J. Minar (LMU München, ZCU Pilsen)

A large number of the material science tasks can be reduced to a rather generic formulation: how to increase an intensity of the useful properties ('signal') or how to reduce the unwanted ones ('noise')? The diversity of the degrees of freedom in polyatomic systems makes such 'signal-to-noise' control rather sophisticated and expensive. In modern technologies, operating on the nanoscale, the requirements for basic elements are often quite stringent: high crystalline order, precise target compositions, etc. Alternative improvements can be provided by disorder. In this context, a desired improvement can be achieved by introducing a specific disorder, suppressing 'noise' intensity, but preserving the intensity of 'signal'. Such engineering requires establishing of the relationships between the 'useful' characteristics, materials structure and particular disorder. Here we would like to assist for a systematic view on alternative adjustment of materials functionalities via manipulating internal degrees of freedom, provided by disorder. We give an overview of various types of disorder and their specifics, methods dealing with disorder explicitly and examples demonstrating the efficiency of such engineering.

Time: Thursday 15:00–17:15 Location: H32

Invited Talk MA 45.1 Thu 15:00 H32

Charge carrier scattering and electronic transport in graphene — •Mikhail Katsnelson — Radboud University, Nijmegen, Netherlands

High electron mobility in graphene is one of its most interesting properties for potential applications. Despite intensive efforts, both experimental and theoretical, we still have no complete understanding of main electron scattering mechanisms and main limiting factors restricting the mobility. It is clear that a long-range scattering is important since short-range scatterers with radius of potential smaller than the electron wavelength are irrelevant for massless Dirac fermions. Three most probable candidates are charge impurities, scattering by elastic deformations created by frozen ripples and other defects, and resonant scattering centers (the last case also deals with long-range effects due to divergence of the scattering length). I review a theory of these mechanisms, together with relevant experimental results and first-principle calculations. I discuss also peculiarities of electron transport in bilayer graphene and temperature dependence of resistivity for freely suspended graphene samples. In the latter case, two-phonon processes involving bending mode give probably the main contribution. I will consider also theory of minimal conductivity in graphene and discuss the role of electron-electron interactions. Electronic transport in graphene on boron nitride and the role of moire pattern formed in this case will be also reviewed.

Invited Talk MA 45.2 Thu 15:30 H32

Electrons in disordered systems: extensions to the coherent potential approximation for short- and long-ranged order effects — •Julie Staunton[1], Alberto Marmodoro[2], and Arthur Ernst[2] — [1]University of Warwick, Coventry CV4 7AL, United Kingdom — [2]Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

The extension of the coherent potential approximation (CPA), namely the Korringa-Kohn-Rostoker (KKR)-nonlocal-CPA method, describes short- and partial long-range order effects on the electronic structure of disordered materials and has been incorporated into a full electronic density functional theory (DFT) and electronic transport formalism. Here we briefly review this method and show how it can be combined with a simple treatment of the statistical mechanics of slowly varying degrees of freedom so that, in principle, an ab-initio theory of phase transitions can be achieved along with descriptions of the development of both short- and long-range order. In this context we use the DFT-based 'disordered local moment' (DLM) picture for magnetism where slowly fluctuating local moments on atomic sites can emerge from the interacting electrons of many materials. Whilst this picture works well for many rare earth and transition metal magnets, fluctuating moments do not establish naturally over such small regions for some materials. We show how the DFT-DLM theory can be extended to these materials with the use of the KKR-NLCPA to allow for more extensive, slow magnetic fluctuations and revisit the description of the paramagnetic states of iron, cobalt and nickel.

15 min. break

Invited Talk MA 45.3 Thu 16:15 H32

Percolation and other models for quenched disorder in materials, and some consequences of this disorder on physical properties. — •Kurt Binder — Inst. of Physics, JGU Mainz

An introductory review of percolation phenomena in solids is given, starting out with the example of diluted ferromagnets, where the spontaneous magnetization vanishes at the percolation threshold already in the ground state. Extensions such as correlated percolation will be mentioned, from clusters in the Ising model to percolation of nanorods in the continuum, emphasizing to understand electrical conductivity. In sodium silicate glasses both the rigid silica network and a network of sodium-rich channels percolate simultaneously, and this feature explains the strong ionic conductivity of these materials.

Invited Talk MA 45.4 Thu 16:45 H32

The Impact of Disorder on Transport in crystalline Phase Change Materials — •Matthias Wuttig — RWTH Aachen

Understanding charge transport in phase change materials (PCM) is crucial to extend the application range of these exciting materials. Hence, we have studied the resistivity of crystalline phase change materials. A pronounced dependence of the room temperature resistivity upon annealing temperature is observed for crystalline PCMs such as Ge1Sb2Te4. This finding is corroborated by low temperature measurements as well as FTIR data, which confirm that a metal * insulator transition is observed without a change in crystallographic state. This is indicative for an electronically driven MIT [1].

Such an MIT can be achieved if the electron correlation exceeds a critical value (Mott MIT). A second route to insulating behavior has been attributed to increasing disorder, which turns a metal into an insulator with localized states. Arguments for disorder induced localization of charge carriers will be presented, which reveal that vacancy ordering drives the MIT [2]. The potential of disorder for applications as well as our fundamental understanding of solids is discussed. [1] T. Siegrist et al., Nature Materials 10, 202, (2011) [2] W. Zhang et al., Nature Materials, 11, 952 (2012).