Disorded Oxides

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Many oxides are use to be reach on various kinds of defects - vacancies, impurities, add-atoms, anti-site defects and other imperfections, which can substantially affect structural, electronics, magnetic, optical, and transport properties of the host material. Some imperfections such as oxygen vacancies or anti-site defects are natural in many systems, while impurities or add-atoms are usually artificially implanted to modify specifically desired properties of a particular system. A design or a study of such materials is a challenge for both experiment and theory. in my talk I present briefly our theoretical approach for the treatment of disorder in oxides and make an overview of our recent related works, many of which were completed in the close cooperation within the current SFB. First, I discuss disorder in ZnO bulk and heterostructures. ZnO is a large band gap non-magnetic insulator and, nevertheless, an important component in many spintronic applications. In various examples I'll illustrate how impurity and defects may induce new functional properties in this material. In particular, due to a spontaneous formation of specific defects and a two dimensional electron (2DEG) gas at ZnO/MgZnO interfaces the anomalous Hall effect can emerge in these non-magnetic systems [1]. I'll present a theoretical model, which explains recent experiments with ZnO/MgZnO heterostructures. As next, I discuss the impact of defects and other imperfections on the formation of a 2DEG at interfaces between two insulators [2,3]. Based on recent experimental results and our numerical simulations we suggest several recipes to tune specific properties of the 2DEG. Finally, I'll present our theoretical model of a metal-insulator transition, which was recently observed in metallic $CaRuO_3$ oxides doped with cobalt [4,5]. We explain the observed reduction of the conductivity in this system at a certain Co concentration using the Anderson localization model, provided that if the degree of randomness in the lattice is sufficiently large, the mean free path of conduction electrons can be strongly reduced.

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