DS 8: Transport Properties

Time: Tuesday 14:00–15:30 Location: REC/B214

DS 8.1 Tue 14:00 REC/B214

Polaron Transport in $BiVO_4$ — •Nils Sekinger[1,2], Tsedenia Zwedie[1,2], and Ian Sharp[1,2] — [1]Walter Schottky Institute, Technical University Munich — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich

Bismuth vanadate ($BiVO_4$) has received considerable attention as a potential photoanode for photocatalytic applications, thanks to its moderate bandgap of ∼2.5 eV and favourable band edge energetics. However, it is believed that photogenerated electrons localise at vanadium sites to form small polarons, while holes localise around BiO_8 units to form large polarons, thereby inhibiting their transport [1]. This study investigates charge transport in monoclinic $BiVO_4$ using temperature-dependent photoconductivity measurements. Under illumination, we observe two distinct thermally-activated transport regimes. With decreasing temperature, the large-barrier electron hopping transport characteristic transitions to a lower barrier regime that may arise from the freeze-out of electron transport, resulting in a dominant influence from minority holes. The transport barriers, hopping distances, and effective masses of both small and large polarons in the dark and with illumination at different intensities are investigated. Analysing the dependence of the resistivity on temperature and light intensity provides critical insights into the polaronic conduction mechanism and offers experimental validation for theoretical models describing polaron transport. These findings improve our understanding of charge transport in $BiVO_4$ and its use in photocatalytic and electrochemical applications.

[1] *Wiktor et al. ACS Energy Lett. 2018, 3(7), 1693-1697*

DS 8.2 Tue 14:15 REC/B214

Correlation of impedance and structural properties in oxides on the microscale — •Jan L. Dornseifer[1,2], Christopher P. Körbächer[1,2], Martin Becker[1,2], Janis K. Eckhardt[2], Matthias T. Elm[1,2], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Germany — [2]Center for Materials Research (ZfM), Jusuts-Liebig-University Giessen, Germany

The charge transport properties of ionically and/or electronically conducting thin films are governed by their elemental composition and microstructure, including their morphology and grain architecture. Electrochemical impedance spectroscopy (EIS) is widely used to probe the electrical properties, yielding macroscopic parameters. However, linking these to the underlying microscopic transport processes requires theoretical models that have so far failed for samples with expansions comparable to their grain sizes.

Here, we present an experimental approach to directly relate impedance, microstructure and microscopic transport properties. Using cerium oxide and vanadium oxide networks with well-defined microscale transport paths, the impedance of individual networks was measured via microelectrodes. Complementary SEM, EDX, and micro-Raman spectroscopy provided detailed structural information. Correlating these data with the impedance offered new insights into the microstructural influences on the charge transport. This represents a promising way to reliably determine microscopic transport properties of polycrystalline thin films on the microscale.

DS 8.3 Tue 14:30 REC/B214

Magnetotransport and Electron Optics in Bilayer Graphene — •Florian Schöppl[1], Ming-Hao Liu[2], Alina Mrenca-Kolasinska[3], Klaus Richter[1], Korbinian Rohrmüller[1], Korbinian Schwarzmaier[1], and Angelika Knothe[1] — [1]Institut für Theoretische Physik, Regensburg, Germany — [2]Department of Physics, National Cheng Kung University, Tainan City, Taiwan — [3]AGH University of Krakow, Kraków, Poland

The remarkable sample quality of bilayer graphene (BLG), combined with the strong electrostatic tunability of its band structure, makes BLG an excellent platform for electron optics. While the system's purity enables ballistic transport on micrometer scales [1,2], trigonal warping near each K point induces a valley-dependent momentum selection, resulting in characteristic anisotropic transport and scattering phenomena [3,4]. To study the interplay between such warping effects and symmetry breaking from gate-defined potentials, we employed quantum-mechanical tight-binding models as well as semiclassical simulations and find pronounced directional conductance in BLG cavities. Motivated by these anisotropic properties, we further analyze unguided -ringless- Aharonov-Bohm configurations and used wave-matching algorithms to tailor electrostatically defined lenses [5] and mirror geometries.

[1] L. Seemann et al., Phys. Rev. B (2023) [2] L. Banszerus et al., Nano Lett. 2016 [3] C. Gold et al., Phys. Rev. Lett. (2021) [4] J. K. Schrepfer et al., Phys. Rev. B (2021) [5] C. G. Péterfalvi et al., New J. Phys. 14 (2012)

15 min. break

DS 8.4 Tue 15:00 REC/B214

Multiscale Simulation of Charge Transport Across Grain Boundaries in Organic Polycrystalline Thin-Film Semiconductors — •Junior-Wilfried Tadjeugue-Nangmo[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technology, Bayreuth, Germany

Grain boundaries (GBs) are known to critically limit charge carrier mobility in organic polycrystalline semiconductors as already used in e.g. organic field effect transistors. In our contribution, we address Technologies with a multiscale computational framework that correlates a GB's morphology with its influence on the charge transport properties. Our approach is, at its core, based on phase-field simulations of grain growth to generate realistic GB networks. Electronic structure calculations then reveal deep trap states and significant energetic disorder at the GB, leading to substantial injection barriers. Charge transfer rates across GBs are then calculated from a hopping model which are finally fed into kinetic Monte Carlo (KMC) simulations to demonstrate the device level influence of GBs. They elucidate the fundamental role of grain boundaries in limiting charge transport and provide critical guidelines for the development of future high-performance organic electronics devices.

DS 8.5 Tue 15:15 REC/B214

Modeling of Indium Tin Oxide Back Contacts in CIGSe Solar Cells — •Oliver Wolf[1], Merve Demir[2], Matthias Maiberg[2], Torsten Hölscher[1], and Roland Scheer[2] — [1]B5 Photovoltaics, Just Transition Center, Martin Luther University Halle-Wittenberg — [2]Photovoltaics Group, Martin Luther University Halle-Wittenberg

Copper Indium Gallium Diselenide (CIGSe) thin-film solar cells achieve high efficiencies >23% on opaque molybdenum (Mo) back contacts (BC). Substituting the molybdenum by a transparent conductive oxide, such as Indium Tin Oxide (ITO), facilitates applications in tandem solar cells or bi-facial configurations, but leads to deteriorated Fill Factors and Open-Circuit Voltages. The origin of the inferior solar cell performance remains unclear, but impeded electronic transport at the rear CIGSe/ITO interface appears most likely, especially in view of thin Gallium Oxide interlayers. To elucidate possible transport mechanisms, temperature-dependent current-voltage (JVT) and capacitance-frequency (CfT) characteristics were performed and analysed by means of numerical simulations with Sentaurus from Synopsys. In the measurements, we observe the occurrence of temperature-dependent kinks in the JVT and steps in CfT, which clearly distinguish the measurements of the solar cells with ITO BC from those with Mo. Based on simulation, tunneling processes turn out to be the dominant transport mechanism at the rear interface. Our results are able to describe the observed performance deficits in CIGSe solar cells with ITO BC.