

## HL 56: New materials and concepts

Time: Friday 11:15–12:30

Location: EW 202

HL 56.1 Fri 11:15 EW 202

**Characterization of dip coated tungsten sulfide flakes** — ●TALHA NISAR, TORSTEN BALSTER, and VEIT WAGNER — Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany  
 $WS_2$  is a promising material for future electronics due to its 2 dimensional nature. In our approach we use growth on liquid surface as an alternative deposition method to atomic layer deposition and chemical vapor deposition to grow tungsten sulfide flakes. For this purpose, ammonium tetrathiotungstate (ATTW) is used as precursor material in a 5 mM aqueous solution. No flakes are formed while at room temperature, formation of flakes at the liquid-air interface is observed after heating the solution at 80°C for an hour. Flakes with sizes up to 50  $\mu\text{m}$  are transferred onto a silicon substrate by dip-coating. A post annealing step is done at 800°C in a quartz tube applying a constant flow of forming gas (95% Ar/5% H<sub>2</sub>) with additional sulfur source. Chemical characterization of the flakes by mean of x-ray photoelectron spectroscopy (XPS) reveal that the flakes initially consist out of WO<sub>2</sub> and ATTW. Post growth annealing converted this layer to WS<sub>2</sub>. High crystallinity of the flakes is proved by Raman measurements.

HL 56.2 Fri 11:30 EW 202

**Nanoporous Alumina Membranes as Promising Platforms for Rationally Designing Supercapacitor Electrodes** — ●HUAPING ZHAO, LONG LIU, YAOGUO FANG, and YONG LEI — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Supercapacitors present growing significance as the advanced energy storage devices to bridge the gap between batteries and conventional capacitors owing to the high power density, the fast charge-discharge rate, and the excellent cycle stability. In addition to the electroactive materials themselves, the design of electrode architectures also plays an important role in determining the charge storage capability and rate capability of supercapacitors. A promising supercapacitor electrode therefore should have larger specific area to realize high charge storage capability meanwhile should provide shorter ion diffusion path and lower electron transfer resistance to enable the achievement of high rate capability. Here, we demonstrate nanoporous alumina membranes as promising platforms for rationally designing supercapacitor nanoelectrodes. By employing nanoporous alumina membranes as nanostructuring templates, supercapacitor electrodes in the forms of arrayed nanorod, nanotube, and nanopore have been designed and fabricated. These as-prepared supercapacitor electrodes have large specific surface area ensuring high capacitance and highly-oriented structure facilitating ion transport, thus high charge storage capability and high rate capability of supercapacitor were achieved simultaneously.

HL 56.3 Fri 11:45 EW 202

**Properties of a novel cubic phase in the monochalcogenides** — ELAD SEGEV, RAN EITAN ABUTBUL, URI ARGAMAN, YUVAL GOLAN, and ●GUY MAKOV — Materials Dept, Ben-Gurion University of the Negev, Beer Sheva, Israel

A new nanometric cubic binary phase has been synthesised in the tin mono-selenide and monosulfide systems,  $\pi\text{-SnSe}$ ,  $\pi\text{-SnS}$ , as cube shaped nanoparticles. This new phase has promising optical properties due to the larger bandgap and non-centrosymmetric structure of the crystal. The structure, atomic positions and band gaps of these phases were determined by ab-initio density functional calculations and found

to be in very good agreement with experimental measurements. The phases were determined to be mechanically stable and energetically close to competing structures such as rocksalt and orthorhombic. Density functional calculations have been extended to study the stability of the new phase in other monochalcogenides systems and new phases are predicted. This talk will focus on the results of our calculations and comparison with experimental studies available. [1] E. Segev et al., A new cubic prototype structure in the IV-VI monochalcogenide system: a DFT study, *CrystEngComm*. 19 (2017) 1751. [2] R.E. Abutbul et al., Synthesis and Properties of Nanocrystalline  $\pi\text{-SnS}$  \* A New Cubic Phase of Tin Sulphide, *RSC Adv.* 6 (2016) 5848. [3] R.E. Abutbul et al., A new nanocrystalline binary phase: Synthesis and properties of cubic tin monoselenide, *CrystEngComm*. 18 (2016). [4] U. Argaman et al., Prediction of the stability of the rhombohedral phase in IV-VI monochalcogenides and its origin, *CrystEngComm*. 19 (2017) 6107.

HL 56.4 Fri 12:00 EW 202

**Strong Anharmonic and Quantum-Nuclear Effects in the Low Temperature Dynamics of CsCl** — ●HAGEN-HENRIK KOWALSKI, MATTHIAS SCHEFFLER, and CHRISTIAN CARBOGNO — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

In solid-state theory, the *quasi-harmonic* approximation is generally expected to hold for the description of the nuclear dynamics in crystals at temperatures  $\ll 300$  K. However, a recent experimental study [1] of single crystalline CsCl reveals that its thermal conductivity is comparable to those of amorphous materials ( $\sim 1$  W/mK). Strong anharmonic effects hence appear to be active even at 50 K, a temperature at which the quantum-statistics for the nuclei is not negligible ( $C_V < 65\%$  of the Dulong-Petit value). Using first-principles calculations, we investigate the nature of these effects by performing fully anharmonic molecular dynamics with *classical* nuclei (MD) and path-integral MD simulations with *quantum* nuclei. The comparison with respective *quasi-harmonic* calculations confirms that pronounced quantum-nuclear and anharmonic effects are active in this material and reveals how the respective mechanisms couple. Eventually, we discuss how these effects can affect simulations of the thermal conductivity [2] and the resulting implications for simulations across material space.

[1] M. Sist, et al., *Ang. Chemie* **56**, 3625 (2017).[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901, (2017).

HL 56.5 Fri 12:15 EW 202

**Scanning tunneling microscopy study of an excitonic insulator candidate** — ●XINGLU QUE<sup>1,2</sup>, LIHUI ZHOU<sup>1</sup>, QINGYU HE<sup>1,2</sup>, TOMOHIRO TAKAYAMA<sup>1,2</sup>, ANDREAS ROST<sup>1,2</sup>, and HIDE-NORI TAKAGI<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for Solid State Research, Stuttgart, Germany — <sup>2</sup>Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany

An excitonic insulator is resulted from strong electron-hole coupling as compared to the single electron energy gap of a semiconductor or semimetal, where new exotic electronic phases have theoretically been predicted to emerge. I present our study of an excitonic insulator candidate by scanning tunneling microscopy. The surface topography as well as the electronic structure was investigated at different temperatures in ultrahigh vacuum. Our atomic resolution studies revealed a strong correlation of its electronic properties with the structure, laying the ground out for further study on physics of excitonic insulators.