Tuneable Work Function of SnO_2 and TiO_2 Nanomaterials: Challenges and Applications

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The work function (φ) of nanomaterials and thin films based on oxide semiconductors (SnO_2 or TiO_2) is one of the key parameters controlling their use in energy applications, such as perovskite photovoltaics, photocatalysis, solar fuel generation and Li-batteries [1]. Yet the determination of φ by photoelectron spectroscopy (XPS, UPS, including NAP-techniques), photocurrent onset potential, Kelvin probe measurements (including KPFM) and electrochemical impedance spectroscopy is challenging, sometimes even impossible for fundamental reasons (e.g. in some nano-porous thin films) [2]. Inconsistent data from various experimental and theoretical works provoked conflicting debate in the literature [3]. We have addressed these contradictions by detailed analysis, tailored materials' syntheses and interface engineering. We found that the work function of ALD-grown SnO_2 is easily tuneable in a broad range of ca. 0.7 eV by the film thickness, calcination or doping (Fig. 1). On the other hand, the work function of ALD-grown TiO_2 is nearly unchanged by calcination, but still markedly smaller than the value of anatase single crystal [2]. Furthermore, TiO_2 thin film is much more sensitive to thermal cracking as compared to SnO_2. This knowledge provides rationale for optimization of oxide semiconductors for various technologies of energy conversion and storage. Acknowledgement: This work was supported by the Grant Agency of the Czech Republic (contract No. 22-24138S).

References

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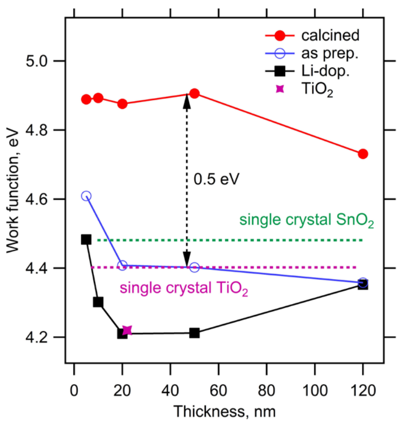

Figure 1: The work function from Kelvin probe measurements on the ALD-grown SnO_2 films of varying thicknesses. Blue: as-prepared (quasi-amorphous) films. Red: calcined at 450ºC in air. Black: subjected to electrochemical doping with Li. The work function of ALD-TiO_2 is shown by magenta star (22 nm film, as prepared or calcined). Green and magenta dashed lines indicate the values for SnO_2 cassiterite (001) and TiO_2 anatase (101) single-crystals, respectively.