Abstract Submitted for the MAR08 Meeting of The American Physical Society

Raman scattering properties of $\mathrm{SnO_x}^1$ RALF MEYER, Theoretical Physics, University of Duisburg-Essen, 47048 Duisburg, Germany, CEDRIK MEIER, AXEL LORKE, Experimental Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — Oxidic semiconductors like $\mathrm{ZnO_x}$ and $\mathrm{SnO_x}$ have recently attracted a lot of attention as possible optical materials for novel technological applications. Results from Raman scattering experiments at $\mathrm{SnO_{1.5}}$ nanoparticles are presented which show strong differences compared to the Raman spectra of bulk $\mathrm{SnO_2}$. In order to understand these differences, ab-initio calculations of the Raman scattering properties of bulk $\mathrm{SnO_2}$ and $\mathrm{SnO_{1.5}}$ have been performed. Raman spectra derived from these calculations compare qualitatively well with the experimental findings. From this, it is concluded that the differences in the experiments are an effect of the bulk materials. An analysis of the nature of the calculated Raman active vibrational modes makes it possible to draw further conclusions on the reasons behind the differences between the stochiometric $\mathrm{SnO_2}$ and the understochimetric $\mathrm{SnO_{1.5}}$.

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