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Local versus global electronic properties of chalcopyrite alloys — RAFAEL SARMIENTO-PÉREZ¹, SILVANA BOTTI¹, ●CLAUDIA S. SCHNOHR², IVER LAUERMANN³, ANGEL RUBIO^{4,5}, and BENJAMIN JOHNSON⁵ — ¹Institut Lumière Matière, Université Lyon 1-CNRS, F-69622 Villeurbanne Cedex, France — ²Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — ³Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — ⁴Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, Avenida de Tolosa 72, E-20018 San Sebastián, Spain — ⁵Fritz Haber Institute, Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

Among the materials used for thin film solar cells, $\text{Cu}(\text{In,Ga})(\text{S,Se})_2$ has reached the highest conversion efficiencies with record values well above 20%. The bandgap energy of the material can be tailored by adjusting the In/Ga ratio which mostly affects the position of the conduction band minimum. Therefore, we have studied the element-specific unoccupied electronic states of $\text{Cu}(\text{In,Ga})\text{S}_2$ as a function of the In/Ga ratio by combining X-ray absorption spectroscopy with ab initio calculations. The S absorption edge shifts with changing composition as expected from the variation of the band gap. In contrast, the cation edge positions are largely independent of composition. This unexpected behavior is well reproduced by our calculations and originates from the dependence of the electronic states on the local atomic environment. The variation of the bandgap arises from a changing spatial average of these localized states with changing alloy composition.

Part: HL
Type: Vortrag;Talk
Topic: Photovoltaik;Photovoltaics
Email: c.schnohr@uni-jena.de