Resonant Inelastic Soft X-ray Scattering of Be Chalcogenides

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Over the last few years it has been shown that information about the bulk band structure can be obtained by resonant inelastic X-ray scattering (RIXS) in the soft X-ray regime. However, conceptual differences exist about the underlying pictures involving keywords such as "resonant X-ray emission" processes, "electronic resonant Raman scattering", and "core exciton formation". To understand and clarify the applicability of the different concepts, we have studied the properties of a new class of materials -beryllium chalcogenides (i.e., BeS, BeSe, and BeTe) – with soft X-ray K_α emission following a resonant Be 1s core hole formation.

Be chalcogenides constitute interesting candidates for several electronic applications of II-VI-semiconductors, e.g., in ZnSe-based blue light-emitting devices or Mn-containing spin aligner systems. We will show that even for such large band gap materials with an indirect gap, the observed spectral variations can be nicely correlated to the band structure derived from accompanying LDA-, EXX-, and GW-calculations taking the involved matrix elements into account. Furthermore, we observe Raman-like inelastic scattering features below the absorption threshold.

Finally, "core excitonic" features above the valence band maximum can be observed for sufficiently high excitation energies. In the case of BeS, we will demonstrate that such information can even be obtained from insulating powder samples. The obtained results will be discussed in correlation with the above mentioned theoretical band structures, in view of the different conceptual approaches, and with a discussion of the underlying physical processes contributing to a loss of k-conservation and the appearance of a major non-coherent fraction in the observed spectra.

The experiments were performed at beamline 8.0 of the Advanced Light Source, Lawrence Berkeley National Laboratory, and funded by the Deutsche Forschungsgemeinschaft through SFB 410, TP B3.