An X-ray Raman scattering study of the Li core excitation spectrum in LiH

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X-ray Raman scattering (XRS) spectroscopy was used to study the Li 1s core excitation spectra in LiH in a wide range of momentum transfers *q*. The analysis of the near-edge region of the measured spectra in combination with *q*-dependent *ab initio* calculations of XRS spectra based on the Bethe–Salpeter equation (BSE) reveals that the prominent peak at the excitation onset arises from two main contributions, namely a pre-edge peak associated to a *p*-type core exciton and strong transitions to empty states near the bottom of the conduction band, which is in contrast to previous experimental studies that attributed that feature to a single excitonic peak. The *p*-like angular symmetry of the core exciton is supported by BSE calculations of the relative contributions to the XRS spectra from monopole and dipole transitions and by the observed decrease of its normalised intensity for increasing momentum transfers. BSE, as well as real-space multiple-scattering calculations, also reproduced spectral features observed at higher energies and their momentum transfer dependence.