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Probing excitonic effects with valence-electron-energy-loss spectroscopy: application to hexagonal boron nitride[1] MYRON KAPETANAKIS[2], Vanderbilt Univ. ORNL, RITESH SACHAN, MARK OXLEY, ORNL, MAUREEN LAGOS, PHILIP BATSON, Rutgers Univ., WILLIAM WEBER, ORNL Univ. of Tennessee, MATTHEW CHISHOLM, ORNL, SOKRATES PANTELIDES, Vanderbilt Univ. ORNL — The interplay between surface and bulk phenomena gives rise to a variety of interesting features, especially for lower-dimensionality systems, and provide the opportunity for the realization of applications in, for instance, optoelectronics and photonics. Such features are triggered by excitonic states that are suppressed at the bulk counterparts of the material. Here we use a combination of monochromated, aberration-corrected scanning transmission electron microscopy (STEM) and density functional theory (DFT) calculations to study the effect of excitons on the valence-electron energy-loss (VEEL) spectra of the wide-band-gap hexagonal boron nitride (hBN). The experimental VEEL spectra are acquired using the state-of-art monochromated aberration corrected Nion UltraSTEM with 8 meV energy resolution. Theoretically, the excitonic effects on the VEEL spectra are understood by solving the Bethe-Salpeter equation (BSE). Within the combined theoretical scheme, we are able to study hBN systems with increasing number of sheets and demonstrate the transition from the pure 2D monolayer to the bulk hBN.

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