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Impurity signatures in two-dimensional materials in atomic-resolution valence-electron-energy-loss spectroscopic maps.¹ MYRON KAPETANAKIS, MARK OXLEY, VANDERBILT UNIV. ORNL, WU ZHOU, JUAN-CARLOS IDROBO, ORNL, SOKRATES PANTELIDES, VANDERBILT UNIV. ORNL — The local atomic configurations and electronic states of impurities in 2D materials can be probed directly by several microscopy techniques. Probes of electronic excitations, however, lack spatial resolution. Here we demonstrate that valence-electron energy-loss spectroscopy in an aberration-corrected scanning transmission electron microscope yields atomic-resolution maps of electronic excitations that provide unique signatures of distinct bonding configuration impurities in 2D materials. We report simulations of the maps based on density functional theory and dynamical scattering theory, which agree with and provide direct interpretation of the observed features. The maps differentiate between different bonding configurations of impurities in graphene and hexagonal boron nitride. The theoretical analysis yields information on local electronic excitations, corresponding to impurity-induced bound, resonant and antiresonant states. The method stands to benefit from new monochromators and detectors that enhance spatial and energy resolution and constitutes a powerful alternative to optical spectroscopies for probing electronic and magnetic signatures related with impurities and defects.

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