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Enhanced transferability for Bethe-Salpeter Calculations ERIC L. SHIRLEY, NIST — We have systematized projector-augmented-wave methods to reliably augment plane-wave/pseudopotential Bloch functions in atomic core regions for purposes of performing screening calculations, evaluating transition matrix elements, and evaluating Slater integrals in the condensed matter environment. This has improved the accuracy of core-hole screening, adherence to sum rules, and control of the strength of absorption features. This also ensures that transition matrix elements and concomitant core excitation spectra are reliable over significant energy ranges. To accomplish this, we improve the quality of the pseudopotentials (which become harder), extending norm conservation, and increasing the number of "valence electrons." We present results for both insulators and metals, and for both core and valence excitations. Comparison to experimental data is a key part of this work. We also emphasize what approximations remain to be tackled in the treatment of electronic excitation spectra, many of which are more difficult to treat than what is within the scope of this work.

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