PAW Calculations for Core Edge Spectroscopy

MICAH PRANGE, WEIDONG LUO, SOKRATES PANTELIDES, Vanderbilt University — The projector augmented wave (PAW) method is the tool of choice for density-functional calculations for bulk materials. Meanwhile, core loss spectroscopies like EELS, XAS, NRIXS, etc. are powerful experimental tools for probing the physical properties of bulk materials. Yet, despite the fact that PAW yields the all-electron Kohn-Sham wave functions, theoretical predictions of core edge fine structure within the PAW method have been limited to projected densities of states (and hence the dipole approximation). We present PAW calculations of full matrix elements of $e^{i\mathbf{q} \cdot \mathbf{r}}$ based on extensions to the VASP code. This strategy provides full-potential near-edge structure at arbitrary momentum transfer. The capability to go beyond the dipole approximation allows applications to spectroscopies for which the signal comes from large $\mathbf{q}$, like NRIXS and EELS in STEM geometry or with an off-axis detector. We compare our results to measurements as well as traditional theoretical approaches.

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