

FEFF6 to FEFF9 expansions of x-ray computational toolbox

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Abstract: FEFF6 ab initio code was successful in replacing earlier empirical standards in EXAFS analysis. This inspired several important expansions for subsequent developments. Spin-dependent calculations for X-ray magnetic circular dichroism became available in FEFF7. Self-consistent muffin-tin potential in FEFF8 was crucial to develop predictive XANES simulations, and making XANES an important addition to structural analysis methods. FEFF9 developments were focused on many body effects in x-ray spectra such as dynamic screening and self-energy. At the same time expansions were made to provide simulation for larger variety of x-ray spectroscopies: emission, DAFS and inelastic scattering. Thus a variety of computational tools were created that are very useful for analysis of various x-ray spectra.