Comparison between calculated LDOS and measured NEXAFS for carbon allotropes and mixtures

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The Local Density of States (LDOS) spectra for different regions carbon allotropes and mixtures are characteristic of the local geometrical structure. After creating carbon samples with specific features (such as vacancies, or graphite/diamond boundaries) we calculate these spectra using the PLATO tightbinding molecular dynamics package, and observe our samples with the AViz atomistic visualization package. AViz enables us to directly observe bond lengths and angles. The NEXAF (Near Edge X-ray Absorption Fine Structure) spectroscopic technique can be used to measure specific bonds and orientations.

In this project we are comparing the calculated LDOS spectra of atoms in specific structures with EXAFS measurements.

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