Austin Houston

Project Proposal

Mse 613

**Background:**

Electron energy loss spectroscopy (EELS) is an advanced scanning transmission electron microscopy (STEM) used to measure chemical bonding, atomic composition, electronic structure, and surface properties of a system. When an electron beam is transmitted through a thin (~100 nm) sample, some electrons are scattered inelastically and lose energy. These electrons are passed through a magnetic field to sort them by energy. The resulting spectra is characterized into three regions: zero-loss peak (elastically scattered electrons), low-loss region (in-elastic scattering from plasmons), and core-loss region (ionization edges corresponding to the excitation of electrons in single atoms). Peaks in the core-loss region broadly elucidate elemental composition while also displaying fine structure called electron energy-loss near-edge structure (ELNES), corresponding to local bonding and coordination.

**Project goal:**

For my PhD thesis, I am focusing on in-situ laser processing of 2D materials in an electron microscope, primarily transition-metal-dichalcogenides. I believe I have produced an undocumented phase in the Pd-Se system, which has a unique structure. These nano-crystal samples are usually so small that the only characterization techniques available are Z-contrast imaging and EELS. For this project, I want to make significant process towards simulating EELS spectra which are reasonably matched to experimental spectra and used to quantify the system. Ultimately, I am hoping to discover what role, if any, carbon plays in this material system.

Again, I am more of a microscopist than a modeler, and I have no experience with DFT, so I have designed this project to have tiered goals. First, I will accurately simulate the near edge structure of carbon. If I can achieve this, I will go on to simulate EELS for different structures in the Pd-Se-C system and attempt to match them to experimentally acquired spectra.

**Relevance:**

The relevance of density functional theory and electron microscopy is ultimately statable in one word: electrons! In all seriousness, this project seems ambitious given my experience with modeling. EELS is inherently an excited state method, and any modeling must account for electron-hole effects. Luckily, I have literature examples to follow. I will experiment with two promising DFT programs: Wein2k (based on (L)APW + local orbitals methods) and CASTEP (based on a plane-wave pseudopotential density functional). The general workflow is shown below:

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**Source/ project guide:**

https://etheses.whiterose.ac.uk/1447/2/phd\_thesis\_seabourne.pdf