Dipole Alignment at the Carbon Nanotube and Methyl Ammonium Lead Iodide Perovskite Interface

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I used mathematical calculations based on density functional theory for ammonia in order to predict what the x-ray spectra would look like for methyl ammonium lead iodide perovskite film, and to understand what each prominent peak on this spectra means. An x-ray spectra is made from detecting ejecting electrons, emitted light, or even a sample current from the target when the x-rays energy meets certain resonance for the targeted material. After completing these theoretical calculations, I found that the material had enough theory to support angular dependent x-ray absorption spectroscopy, meaning that I would measure different detected measurements for different angles of the x-ray, where other materials are invariant to this change if there were no dipole alignments. In the experimental x-ray absorption spectroscopy, the perovskite without carbon nanotubes did not have any angular dependence, which suggests that the dipoles within the material are not aligned; however, adding the carbon nanotubes on top of the perovskite did have angular dependence. The alignment could not be determined because the carbon nanotubes had nitrogen sources inside of it, such as pyridine, which had resonant energies and detect measurements dominating over the regions of interest. More work will need to be done to determine valid ways of removing these dominating measurements, but the changes noticed between no carbon nanotube and with carbon nanotube, as well as pyridine, gives insight on factors that might control the dipole's alignment.