



Figure 1: Experimental XPS O 1s for LaNiO₃ surface data plotted with two peaks one at 531.1 eV and one at 528.3 eV. The second graph depicts the spectra of the surface without adsorbed species and last four graphs show the spectra of the adsorbed species and the effects of the adsorbed species on the nearby surface atoms. On the right: Images of species contributing to each of the peaks in the presence of adsorbed atoms/molecules. The border color corresponds to the energies marked on the theoretical XPS graph. Spin up and spin down Ni are shown in black and grey respectively. The corresponding atoms are circled in white.