

Figure 1: Adsorption of CO<sub>2</sub> on LaFeO<sub>3</sub> in a bidentate configuration. The coverages range from ¼ ML to 1 ML with energies below each case.

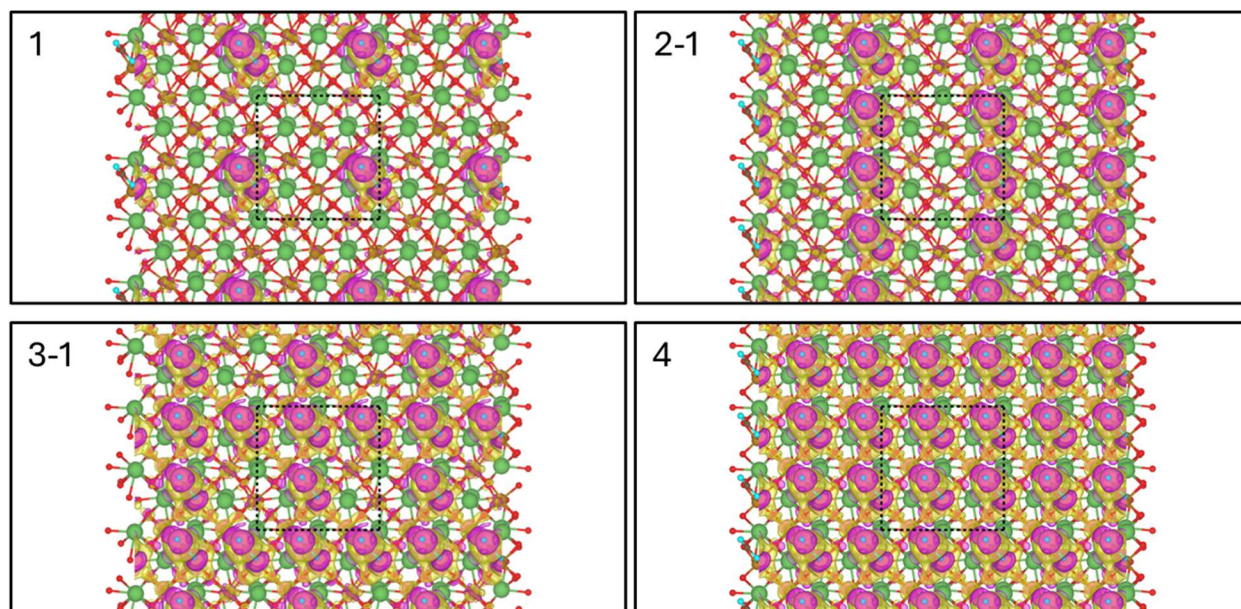


Figure 2: Charge differential analysis with an isosurface of 0.0008 electrons/Bohr<sup>3</sup>. Charge gain is marked with yellow and charge loss is marked with pink. Charge can be seen travelling through the interstitial oxygen while the direct interactions between CO<sub>2</sub> is absent.