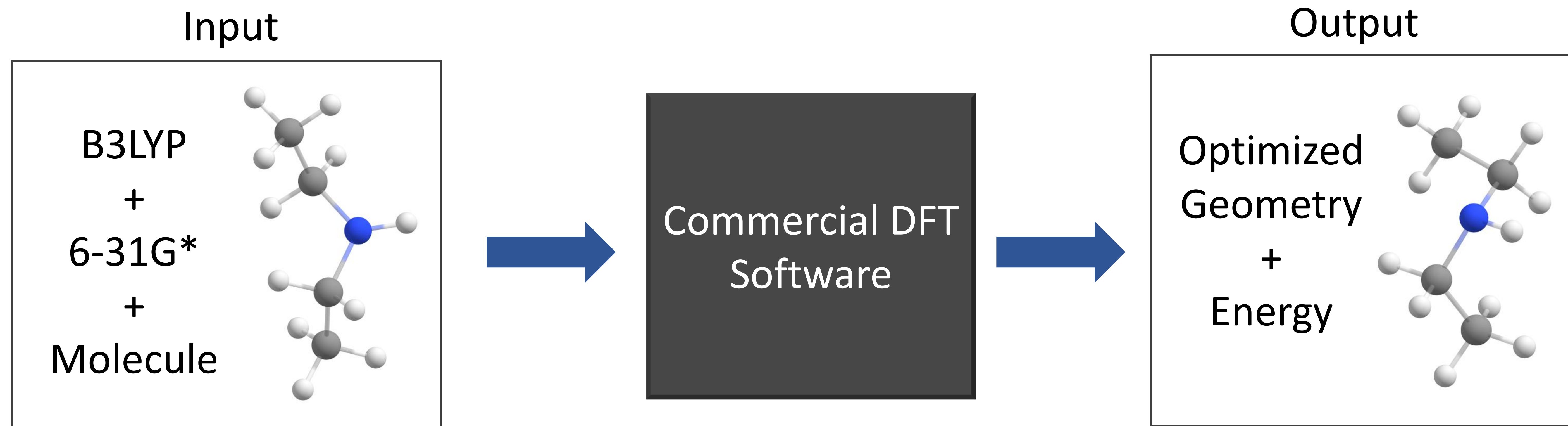
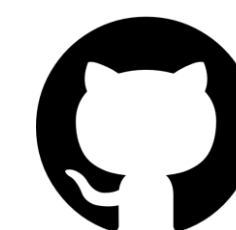


a)

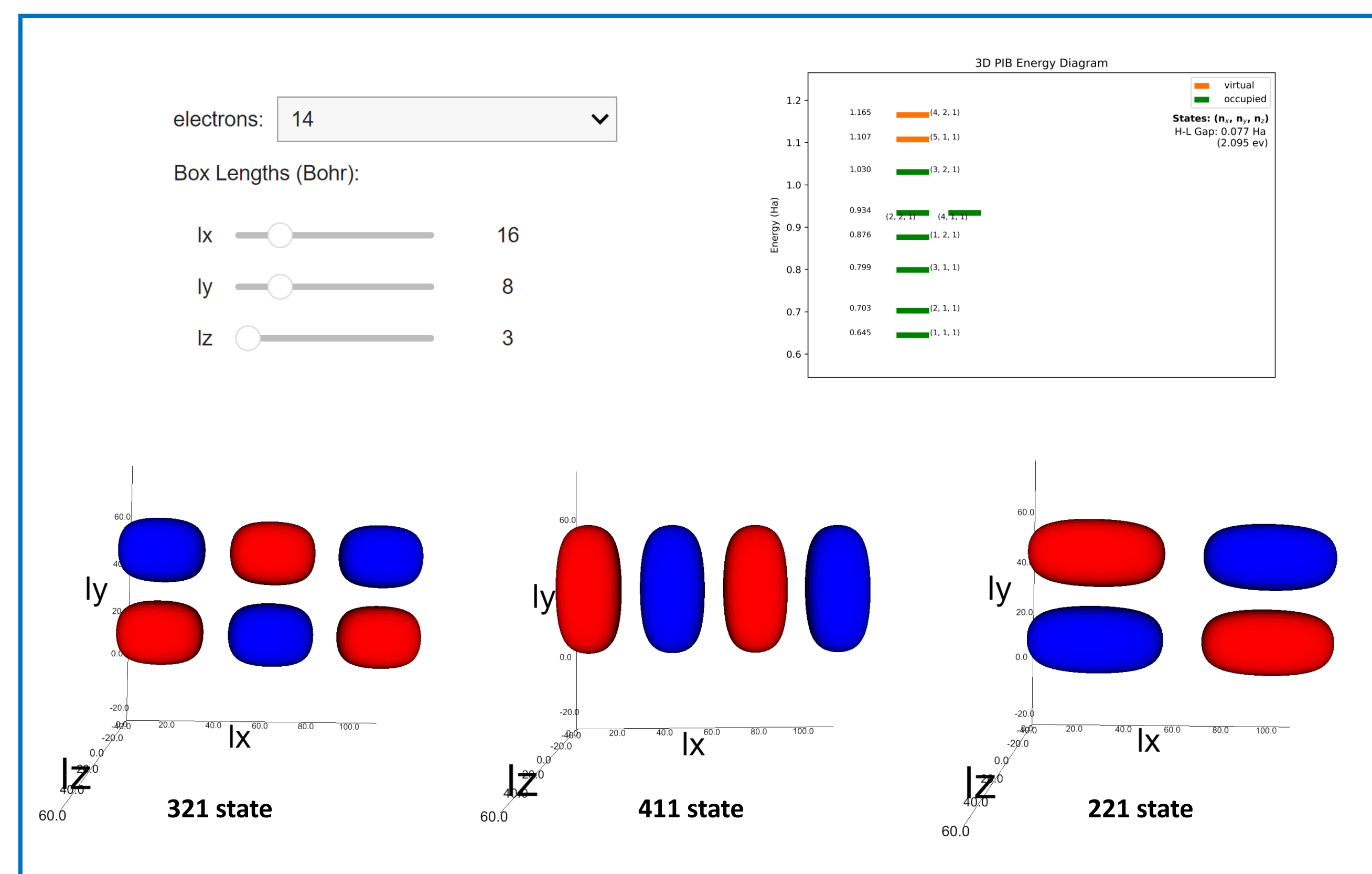


b)

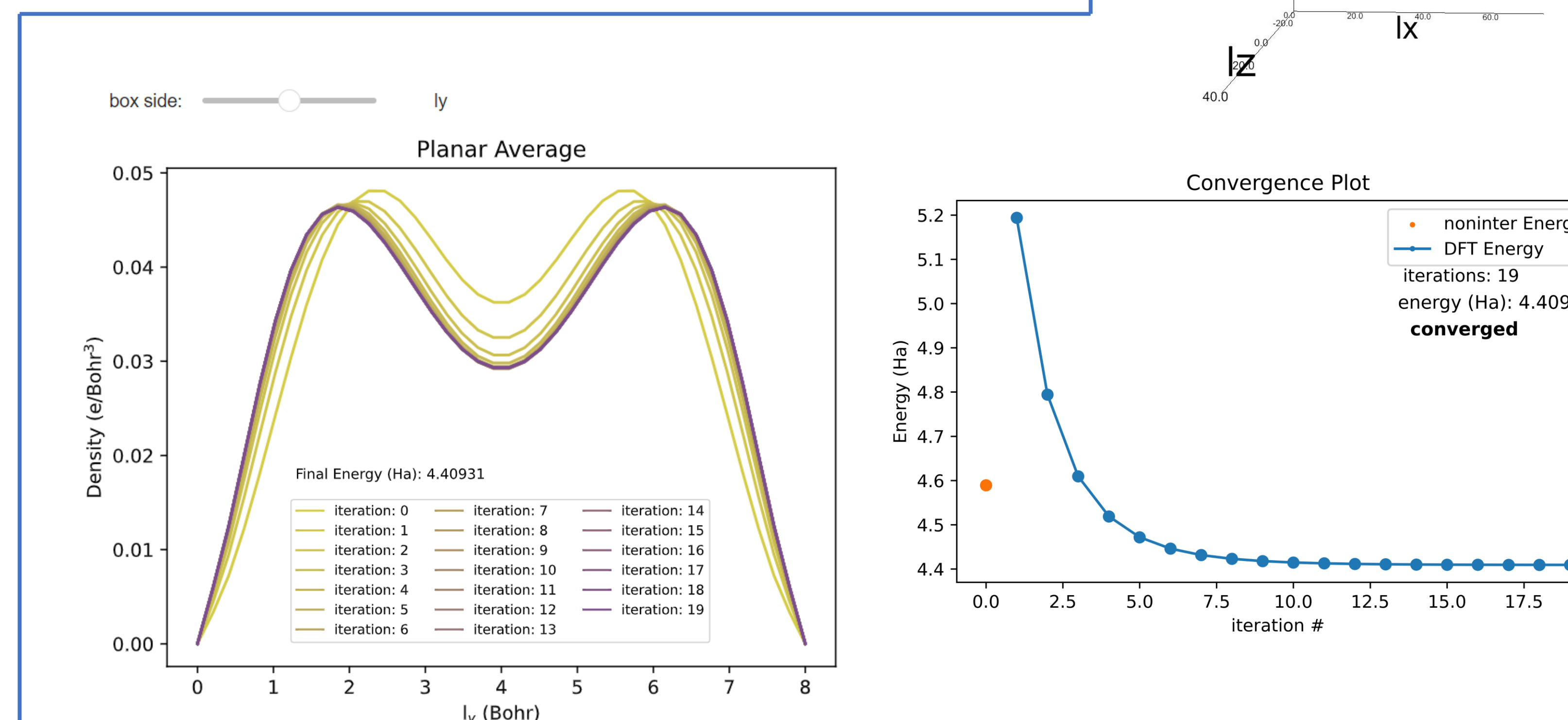
Open-Source Pedagogic DFT Software!



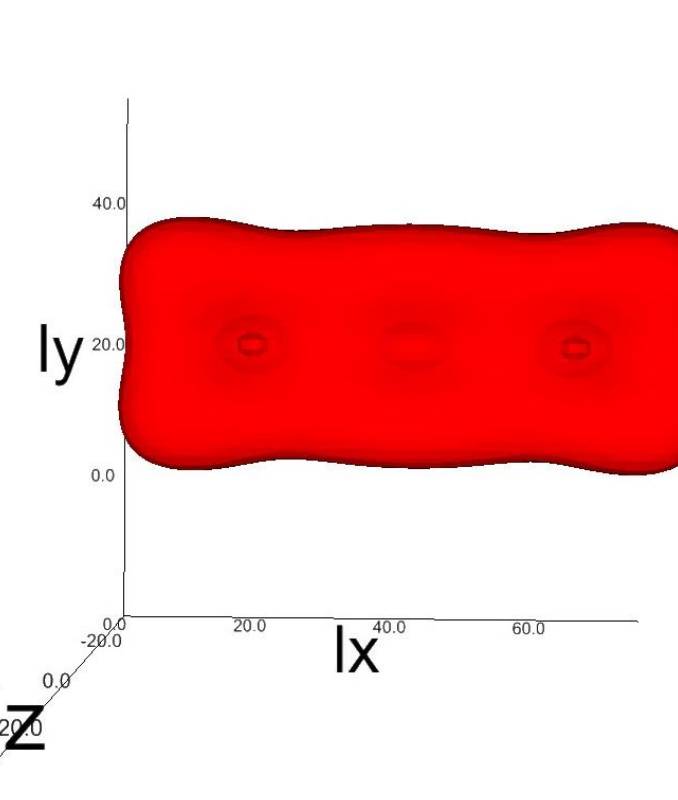
3D PIB Notebook



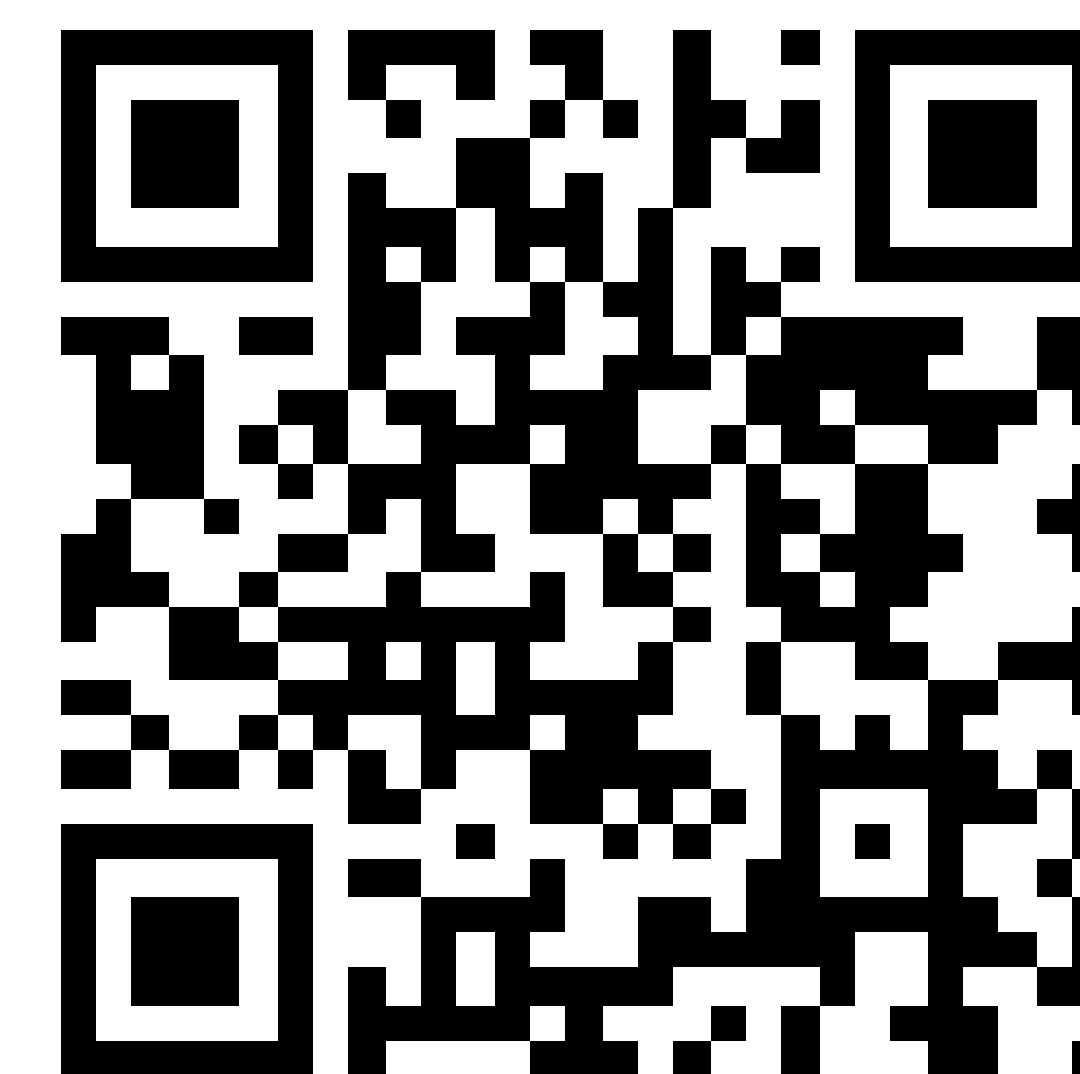
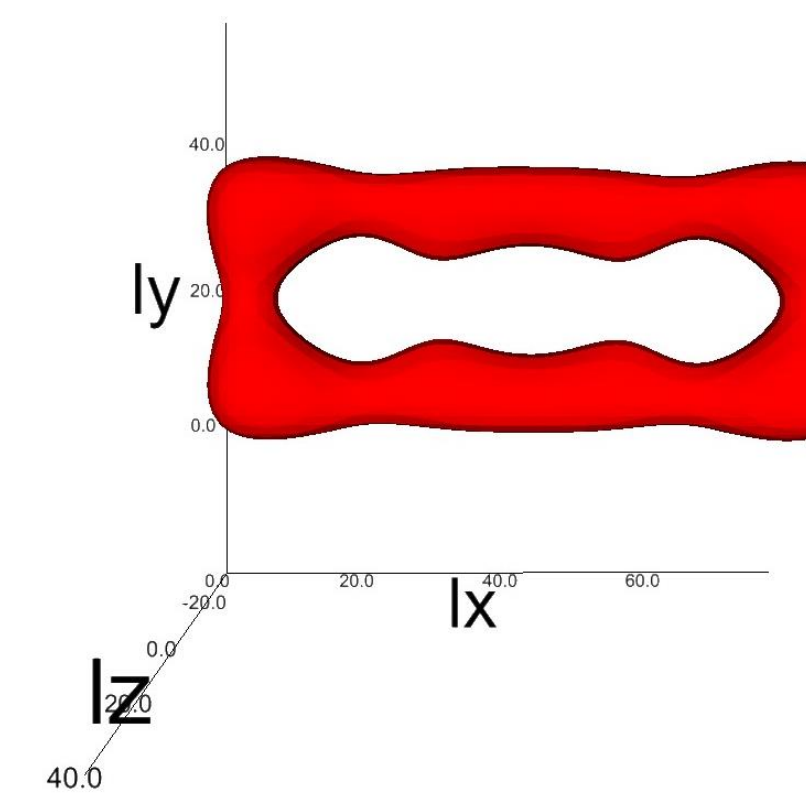
DFT-PIB Notebook



=====
Electron density @ iteration 0
=====
isovalue: 0.06479 e/Bohr**3



=====
Electron density @ iteration 19
=====
isovalue: 0.06479 e/Bohr**3



github.com/tjz21/DFT_PIB_Code

a) Most users of commercial electronic structure packages interact with DFT as a black box method. b) To help remedy this knowledge gap, we have developed three Jupyter Notebooks¹ that explain the fundamentals of DFT through a 3D particle in a box model system with interactive visualizations.