Challenge Kickoff 2018
Introduction to Machine Learning in Materials Science
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Demonstration I (Copper)

1. Open Copper.vesta
    a. Go to Edit -> Edit Data -> Unit cell
    b. Write Down the values for Lattice parameters (the first row)
    c. Go to Structure Parameters and write down the coordinates for Copper (Cu)
    d. Count the number of corner Atoms
    e. Count the number of face atoms
    f. Number of atoms in this unit cell =

Demonstration II (PVDF)

1. Open PVDF_TFP.vesta
    a. How many atoms in unit cell?
    b. What is the crystal structure?
    c. Estimate the C-C, C-F, C-H bond lengths and bond types.
    d. What's the drawback of this model representation? (Hint: Is it crystalline?)
    e. List the electro negativities of C, F and H.
    f. What property you can perhaps estimate just from these given information?