Tutorial – 2

MTN – 316: Materials Informatics

1. Create a dataset of all the binary and ternary oxides of 13^{th} group elements (B, Al, Ga etc.) containing following properties,

   a. Chemical formula
   b. Lattice parameters (a,b,c, α, β, γ)
   c. Density
   d. Formation Energy / Atom
   e. Energy Above Hull / Atom
   f. Band Gap

2. Plot the histogram and box plots for all the properties in the dataset.

3. Comment on the distribution and scales of different properties.

4. Find out any missing or outlier values in the data set and treat them appropriately with proper justification.

5. Compare different scaling options and comment on the most suitable one.