- **Download and install a recent version of the QuantumESPRESSO distribution**

  (visit www.quantum-espresso.org → download → gitlab)

  Input data description available at www.quantum-espresso.org → resources → documentation → input data desciption

- **Select one (not yet selected) element in the Transition Metal Series and insert your name in the ELEMENTS file in the shared Dropbox directory.**

- **Download the corresponding PBE pseudopotential (uspp or paw at your choice) from the Pslibrary-1.0.0 distribution**

  (visit www.quantum-espresso.org → pseudopotentials → PSlibrary)

- **Determine the *ecutwfc* and *ecutrho* needed to converge the total energy to 1mRy/atom in the FCC structure**

- **Compute the structural properties of the selected element in the FCC, BCC and HCP structure paying attention that BZ sampling is accurate well within 1 mRy/atom.**

- **Write a short report on your findings and upload it on the Dropbox repository** **DUE DATE Fri Nov 23rd**