

CSCI699 Assignment 2 — Make Your Own PAW Pseudopotentials

Due: Wednesday, March 7, 2018

Construct a projector-augmented wave (PAW) pseudopotentials for the 5d, 6s and 6p orbitals of tungsten (W, atomic number $Z = 74$) using the ATM program in the class GitHub repository, https://github.com/USCCACS/QXMD_Course.

Submit the following plots, based on discussions in Sugahara *et al.*, *Phys. Rep. Kumamoto Univ.* **12**, 279 (2006) [<http://cacs.usc.edu/education/cs699/SugaharaUSPP-Kumamoto06.pdf>].

1. All-electron and pseudo wave functions as a function of radius for each of the three angular momenta (5d, 6s, 6p).
2. Estimated error as a function of the cutoff energy E_{cut} for pseudowave functions, *i.e.*, Eq. (4.1) in Sugahara *et al.*
3. Fourier components of the augmentation functions for the three angular momenta as a function of the cutoff energy $E_{\text{cut}}^{\text{dens}}$ for the electron density, *i.e.*, Eq. (4.3) in Sugahara *et al.*