The JTH PAW data table

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In this talk, we shall present the way the JTH PAW data table has evolved since its first publication [1], We shall detail the different improvements that have been carried out, especially the way it is tested. In peculiar, we shall show that it is necessary to have a large All Electron data base to validate the PAW data, more extended than the Δ factor one. We shall discuss the XML common format and some numerical problems we had to solve.

References

[1] F. Jollet, M. Torrent, and N. Holzwarth. Generation of projector augmented-wave atomic data: a 71 element validated table in the XML format. *Comp. Phys. Comm.*, 185:1246–1254, 2014.