

Convergence tests for `Mn.pbe-sp-van_mit.UPF`, courtesy of D. Ceresoli and E. Li.

This ultrasoft pseudopotential has been generated in the Mn 2+ configuration (3d4.5 4s0.4 4p0.1), with uspp-7.3.6, and converted to UPF. This pseudopotential has been tested successfully on simple solids (Mn-fcc, MnO) as well as on some Mn organic complexes.





