MBK2013/ATK

Morrison-Bylander-Kleinman 2013 NCPP dataset / ATK 2015

name and version of the code: ATK 2015
type of basis set: pseudo-atomic orbitals
method: norm-conserving pseudopotentials (Morrison-Bylander-Kleinman 2013)

GENERAL INFORMATION

exchange-correlation functional
relativistic scheme
assignment of core / valence states
basis set size
k-mesh density
reciprocal-space integration method

METHOD-SPECIFIC INFORMATION

ADDITIONAL COMMENTS

No supplementary information available.

REFERENCES