ONCVPSP(SG15)2/ATK

SG15 ONCVPSP 2015-05-20 NCPP dataset / ATK 2016

name and version of the code: ATK 2016 type of basis set: pseudo-atomic orbitals

method: norm-conserving pseudopotentials (Schlipf-Gygi ONCVPSP 2015-05-20)

GENERAL INFORMATION

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

METHOD-SPECIFIC INFORMATION

ADDITIONAL COMMENTS

No supplementary information available.

REFERENCES