

FHI-aims/light

FHI-aims 081213 / NAO light

name and version of the code: FHI-aims 081213

type of basis set: numeric atom-centred orbital basis functions

method: all-electron

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