



Contribution ID: 224

Type: Young Crystallographers Lightning Talks(+poster)

A Periodic Density Source for a Periodic System: Using PAW-DFT for Hirshfeld Atom Refinement

Wednesday, 16 March 2022 17:36 (20 minutes)

Previous Hirshfeld Atom Refinement approaches have used non-periodic calculations in order to obtain atomic form factors. We have implemented HAR on the basis of periodic PAW calculations and want to present details and results of this new approach.

Primary author: RUTH, Paul Niklas (Institute of Inorganic Chemistry, University of Göttingen)

Co-authors: Prof. STALKE, Dietmar (Institute of Inorganic Chemistry, University of Göttingen); Dr HERBST-IRMER, Regine (Institute of Inorganic Chemistry, University of Göttingen)

Presenter: RUTH, Paul Niklas (Institute of Inorganic Chemistry, University of Göttingen)

Session Classification: Postersession

Track Classification: Young crystallographers Lightning Talks