

Abstract Submitted
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Distorted plane waves - new basis set for the interstitial region

FREDRIK BULTMARK, Uppsala University — In the LAPW method plane waves are used to describe the wave function and charge density in the interstitial region between the muffin tin (MT) spheres. Plane waves are an excellent basis set for the interstitial region in many aspects - they have a well defined energy and simulate well the charge density of many materials. However in many applications the number of basis functions needed to describe the wave functions and charge density to desired precision is quite large and the diagonalisation of the corresponding Hamiltonian will be time consuming. In order to speed up the diagonalisation and make it possible to perform calculations on larger systems we implement a new set of basis functions, the distorted plane waves which conserves the simplicity of the plane waves, but reduce the number of basis functions needed to describe the wavefunctions to desired precision.

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