Software Spec - MattheissMuffinTin

Implements the Mattheiss prescription for creating muffin tin potentials by overlapping charge densities.

New(cluster, atomid, Nshells, optional Rmt)

Theory (following <http://hermes.phys.uwm.edu/projects/elecstruct/mufpot/MP/MP.Theory1.html>)

We begin with the set of free atom radial wave functions taken from Herman and Skillman. For a closed subshell (electron occupancy ), the (spherically symmetric) electron density can be written

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This is normalized by the condition (extra factor of 2 due to electron spin)

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Where is the number of electrons in the subshell. The total electron charge density due to all electrons in the atom is

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The point of the process is to construct the potential arising from the nuclear charge, the electron cloud, and any overlapping charge from nearest-neighbor atoms.

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Where is the potential due to the charge density , found by solving the Poisson equation:

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Since and depend only on the radial coordinate, we need only the radial part of the Laplacian:

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And thus Poisson’s equation becomes:

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For a given density, this equation can be solved for the potential.

The next step is to superimpose the spherically-symmetric potentials of neighboring atoms to find the muffin-tin potential at any particular atom. We do this by expanding the potential for atom n about the origin (assumed to be at the center of the muffin-tin atom) in terms of spherical harmonics:

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The zeroth order spherically symmetric component of the potential of atom n referenced about the origin (at a distance a from the origin) is:

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And therefore the total spherically symmetric coulomb potential of the muffin-tin is

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Where is the distance from the origin of the muffin tin to the origin of the nearest-neighbor atom n (bond distance).

In a similar fashion, contributions to the Slater exchange potential due to nearest-neighbor atoms will be

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And the total spherically symmetric potential of the muffin-tin, including exchange, is

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Practical implementation:

As increases, the relative contribution to the central potential decreases rapidly. In practice it should not be necessary to sum over more than 1 or 2 nearest-neighbor shells. Potentials derived by this method will be site-dependent, especially in that surface atoms will have a different potential than bulk, which gives a better approximation of reality than Pendry muffin-tin potentials.

Requirements:

1. Need a list of nearest neighbor radial distances and chemical species
   1. Flyweight for chemical species free atom objects.
   2. SortedList on radial distance from atom of interest. Would be nice to have a structure that organizes the list into shells and
2. Atoms need to expose functions to retrieve V(r) (without exchange) and rho(r)
3. OR – only expose rho(r) and use that to compute potentials using Poisson’s equation.
   1. Downside – ATOM already stores potential internally. It would be simple to factor out the exchange piece to return V(r) sans exchange.

Class AtomicPotential

V()

Rho()

Mesh()

VSansExchange()