Opium Generated Pseudopotentials

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The proper design of augmentation operators governs the differences in total energies between test configurations of OPIUM generated transition metal pseudopotentials. The transferability of these d block metal pseudopotentials, between neutral and highly ionized states, is vastly improved if the non-local potentials are designed according to the trends presented herein. There seem to be two clear trends in designing accurate transition metal pseudopotentials that contain an augmentation operator. Early transition metals with a slightly repellant augmentation operator require a maximally ionized semi-core reference state to closely match bulk physical properties. Later transition metals, which are only slightly ionized, require an attractive augmentation operator to match bulk metal properties. All transition metal pseudopotentials as well as their accompanied physical tests have been published online under the Rappe Group's website[1].

[1] http://lorax.chem.upenn.edu/Research/index.html