

Accurate construction of transition metal pseudopotentials

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Abstract

We use the Designed Nonlocal procedure of Ramer and Rappe to examine the effect of pseudopotential transferability on solid state results. We find that lattice constants and bulk moduli are much more sensitive to pseudopotential construction errors than previously thought. We also examine the criteria used to construct accurate transition metal pseudopotentials. We find that both the preservation of all-electron derivative of norm with respect to filling and the preservation of all-electron derivative of eigenvalue with respect to filling are necessary to give good bulk metal lattice constant and pseudopotential. We show how the wide range of lattice constant and bulk modulus results found in the literature can be easily explained by pseudopotential effects.