

Abstract Submitted  
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**An Evaluation of the Rigid Band Model and the Virtual Crystal Approximation in the Transition Metals**<sup>1</sup> DIMITRIOS PAPACONSTANTOPOULOS, FRED IACOLETTI, ALEX KOUFOS, George Mason University — The Schrodinger equation was solved using the Augmented Plane Wave (APW) Method for transition metals in both the body centered cubic (bcc) and face centered cubic (fcc) structures. This method accurately predicts the equilibrium lattice parameter and the ground state of all transition metals. The Rigid Band Model tests based on the group eight and group nine transition metals was applied to predict the density of states (DOS) at the Fermi level for the rest of the transition metals. This test agreed with direct calculations quite well with only a few exceptions in the hexagonal structures. The APW method was also applied using the virtual crystal approximation to obtain the DOS of binary alloys. The results will be compared with direct calculations of ordered and disordered structures.

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