

COMPARISON OF THE CALCULATED SURFACE ENERGY OF METAL USING PSEUDOPOTENTIAL MODEL WITH OTHER CALCULATED METHODS AND EXPERIMENTAL VALUES

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ABSTRACT

The Surface energy γ is the surface free energy per unit area of a particular crystal. The low index surface energies of metal surface was calculated for sixty (60) metals in the periodic table using the pseudopotential model proposed by Perdew(1995). The results obtained were compared with the Full Charged density (FCD), Full Potential calculation as well as the Experimental Values. Results obtained shows that the calculated results agreed well with the other works as well as experimental values.

KEYWORDS: Metal Surface Energy, Fully Charged Density (FCD), Full Potential (FP), Psuedopotential Model (SJM)