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Structural Stability of Crystalline Compounds

Global surveys of material properties have attracted
much interest in recent years. The problem which has
been analyzed in most detail is the mapping of crystal
structures of simple binary AB compounds using
phenomenological coordinates. ' 5 On the other hand, an interesting microscopic model of the complex fami-
ly A = (d transition metal), 8 = (p nontransition met-al) (containing about 200 compounds), which success-fully separates crystal structures, has recently been
presented6 in this journal by Pettifor and Podloucky
(PP). Excluded from their discussion are compounds where 8 =first-period or s metal.
The relative merits of microscopic and phenomeno-logical global surveys are to some extent a matter of taste. Because of the small energy differences between crystal structures one might believe that a tight-binding framework such as that used by PP, which cannot predict equilibrium volumes accurately, would not adequately predict structural energy differences. One instead would expect that self-consistent calcula-tions using a convergent basis set would be necessary. 7 Nevertheless, PP argue that for p-d compounds the p and d atom core repulsive interactions are qualitatively
different. This difference, supported by parametrized
band energies, explains most of the observed structur-al patterns.
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