**Computational Study of High Entropy Alloys For Biomedical Applications**

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High entropy alloys (HEA) has attracted a great attention recently due to many potential new applications especially in bio-medical areas. However, the fundamental theory and reliable modeling of HEA are still not fully developed. Here, we present a new approach that is quite different from existing approaches. The idea is to build large supercells of random solid solution models for HEA and perform detailed DFT calculations on the electronic structure, interatomic bonding and partial charge distributions to provide critical parameters, total bond order density (TBOD) and partial bond order density (PBOD). Results on the application of this new approach to six BCC biofunctional HEA in models of 250 atoms in equal atomic compositions will be presented and discussed. They are: TiNbTaV, TiNbTaZr, TiNbTaZrMo, HfNbTaV, NbTaTiVZr, and TiZrHfNbTa. It turns out that TiNbTaV has the highest TBOD and TiZrHfNbTa has the smallest. Also calculated are the elastic and mechanical properties.

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