



Theoretical design of single phase high-entropy alloys

By Fuyang Tian

LAP Lambert Academic Publishing Dez 2017, 2017. Taschenbuch. Condition: Neu. Neuware - High-entropy alloys (HEAs) form a new class of materials, and show great promises for various demanding engineering applications. Since 2004, many experimentalists worked on HEAs to understand their microstructure and the mechanisms behind the observed excellent mechanical behavior. Ab initio calculations have demonstrated their power in modeling and designing functional materials. Despite of that, the search for new HEAs has still remained heavily dependent on experiments only due to the complexity of modeling multicomponent solid solutions from first principles. Starting from year 2011, Tian et al. used an efficient ab initio alloy theory formulated within the exact muffin-tin orbitals method, to investigate the fundamental properties of HEAs. Their goal is to predict new HEAs with optimal characteristics and identify potential application areas. 84 pp. Englisch.



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