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New Generation Structural Materials: Ab initio Based Modeling of High-Entropy Alloys G. MALCOLM STOCKS, XING-QIU CHEN, EASO P. GEORGE, CHONGLONG FU, TAKESHI EGAMI, Oak Ridge National Laboratory, Division of Materials Science and Technology, MATERIALS THEORY TEAM — There is rapidly growing interest in a new generation of structural materials called high entropy alloys. This class of alloys is multi-component ($\sim$ five elements) with approximately equiatomic ratio, and thus have high entropy of mixing by which they are distinguished from conventional alloys. It has been reported experimentally that the single bcc-based AlCoCrFeNi, single fcc-based CoCrCuFeNi and FeCrMnNiCo high-entropy alloys exhibit promising mechanical properties with potential applications. In this work, we introduce ab initio based modeling for understanding structural, magnetic, and elastic properties based on relaxation of randomly generated supercells within the framework of density functional theory. We studied component-dependent phase stabilities, electronic structures, and magnetic properties with all solutes at fixed and relaxed positions. The properties are analysed in terms of the underlying electronic structure and suggestions are made for further experimental studies to further clarify the reasons for the unusual stability of these systems. Research sponsored by the Division of Materials Science and Engineering, Office of Basic Energy Sciences, U.S. DOE.

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