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An ab initio study of the crystal structure of the Tau-phase in Al-Mg-Zn alloys LAALITHA LIYANAGE, JEFFREY HOUZE, SUNGHO KIM, MARK HORSTEMEYER, SEONG-GON KIM, Center for Advanced Vehicular Systems, Mississippi State University — Existing crystal structures for the intermetallic Tau-phase in Al-Mg-Zn alloy are studied by density functional theory calculations using projector augmented wave pseudopotentials. Favorable crystal structures are identified through volume optimization and formation energy calculations. Properties such as elastic constants and bulk modulus of the crystal structure are determined.

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