

Abstract Submitted  
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**Giant Magnetostriction of Fe-based alloys with an addition of 5d (Ir and Pt) element**<sup>1</sup> YANNING ZHANG, RUQIAN WU, University of California, Irvine — Extraordinary large magnetostriction recently found in Fe-based alloys such as Fe<sub>1-x</sub>Gax (Galferol), continues to attract extensive research interest because of their potential for broad application. To provide clear understanding of the mechanism and also to make rational predictions, we performed full potential linearized argument plane-wave calculations for ternary alloys with the addition of 5d elements (Ir and Pt). In several hypothetical structures, these alloys may have giant tetragonal magnetostrictive coefficient because of the combination of strong magnetization of 3d atoms and the large spin-orbit coupling of 5d atoms. For example, we found that  $\lambda_{001}(\text{Fe}_{75}\text{Pt}_{6.25}\text{Ge}_{18.75})$  is as large as -3553ppm. These predictions indicate that ternary alloys can be attractive smart materials and experimental verifications are underway. We will discuss the preferential distribution pattern of 5d and metalloid elements, spin density features, and inter-atomic hybridization in these alloys so as to provide insights for further experimental explorations.

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