

Abstract Submitted  
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**Enhanced Icosahedral Order in Supercooled Liquid Iron** P. GANESH, MIKE WIDOM, Carnegie Mellon University — As part of a study of metallic glass-forming ability, we perform first-principles molecular dynamics simulations of supercooled liquid Iron. Analyzing the results according to the icosahedral order parameter  $\hat{W}_6$ , we find that Iron exhibits enhanced icosahedral order compared with supercooled Copper and compared with dense random packing. Voronoi analysis confirms the enhanced order is in the form of 13-atom icosahedral clusters as well as characteristic Frank-Kasper type disclinated icosahedra. Upon further cooling the sample crystallizes to a BCC lattice, with the icosahedra clustering to form a novel point defect.

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