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Analysis of Amorphous Iron Surface Energies and Bulk Properties using DFT[1] CHARLES NEWNAM, U.S. Naval Academy, MICHAEL MEHL, U.S. Naval Research Laboratory, DANIEL FINKENSTADT, U.S. Naval Academy — From Ab Initio calculations, we compare the energy of amorphous Iron to bcc and fcc Iron structures, both at zero pressure and high pressure. From these calculations we draw conclusions on the properties of metallic glass structures over a range of pressure. Additionally, we address the adsorption energy of Oxygen on amorphous surfaces versus the structure's cell size and compared against bcc and fcc Iron structures. The adsorption energies allow us to evaluate the corrosion potential of an amorphous structure versus a typical crystalline surface.

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