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Large and realistic models of amorphous silicon[1] DALE IGRAM, Ohio University, BISHAL BHATTARAI, Washington University in St. Louis, PARTHAPARATIM BISWAS, The University of Southern Mississippi, DAVID DRABOLD, Ohio University — Amorphous silicon (a-Si) models are analyzed for structural, electronic and vibrational characteristics. Several models of various sizes have been computationally fabricated for this analysis. It is shown that a recently developed structural modeling algorithm known as force-enhanced atomic refinement (FEAR) provides results in agreement with experimental neutron and X-ray diffraction data while producing a total energy below conventional schemes. We also show that a large model (∼500 atoms) and a complete basis is necessary to properly describe vibrational and thermal properties. We compute the density for a-Si, and compare with experimental results.

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