Abstract Submitted
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Fluid $Fe_{(1-x)}H_x$ under extreme conditions[1] ALEXANDRA SECLAMAN, Ludwig Maximilians Univ, HUGH F. WILSON, RMIT University, RONALD E. COHEN, Extreme Materials Initiative, Geophysical Laboratory, Carnegie Institution for Science Ludwig Maximilians Univ — We study the fluid Fe-H binary system using first principles molecular dynamics (FPMD) and a new FPMD-based method, CATS, in order to compute efficiently and accurately the equation of state of Fe-H fluids up to 5 TPa and 30,000K. We constructed GRBV-type LDA pseudopotentials for Fe and H with small rcuts in order to avoid pseudo-core overlap. In the liquid Fe regime we find good agreement with previous works, up to the pressures where data is available. In the high density regime of pure H we also find good agreement with previous results. Previous work has been focused on low Fe concentrations in metallic liquid H. We extend previous studies by investigating several intermediate $Fe_{(1-x)}H_x$ liquid compositions, as well as metallic liquid H and Fe. Preliminary results indicate extreme compositional pressure effects under isothermic and isochoric conditions, 3.9 TPa difference between Fe and H at 20,000K. Thermal pressure effects are comparatively small, 0.12-0.15 TPa per 10,000K for H and Fe, respectively. Equations of state will be presented and fluid immiscibility will be discussed.

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