

MAR17-2016-000121

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Supercooled water: three-body interactions, IR spectra in no man's land, and the liquid-liquid critical point

JAMES SKINNER, University of Wisconsin

No man's land is the region in the metastable phase diagram of water where it is very difficult to do experiments on liquid water because of homogeneous nucleation to the crystal. There are a number of estimates of the location in no man's land of the liquid-liquid critical point, if it exists. We suggest that published IR absorption experiments on water droplets in no man's land can provide information about the correct location. To this end, using our simulation model with explicit three-body interactions, we calculate theoretical IR spectra for liquid water over a wide range of temperatures and pressures, and use the results to argue that the temperature dependence of the experimental spectra is inconsistent with several of the estimated critical point locations, but consistent with others.