Abstract Submitted
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First-principles simulations of planetary ices S. HAMEL, A. CORREA, Lawrence Livermore National Laboratory, M. BETHKENHAGEN, University of Rostock, R.N. MULFORD, Los Alamos National Laboratory, D.C. SWIFT, Lawrence Livermore National Laboratory — A large fraction of the transiting exoplanets observed are similar in mass and radii to the Ice Giants in our Solar System. The structure of such planets is heavily dependent on the equation-of-state properties of mixtures of water, ammonia and methane (referred to as "planetary ices") at high pressures and temperatures. Many observables properties of Uranus and Neptune, such as gravitational moments and magnetic fields, are thought to be determined by the physical and chemical properties of matter within this ice layer. Of particular interest is the impact of the complex organic chemistry on the fluid properties at these extreme conditions. To cover the wide range of pressure and temperatures relevant to the description of these planets, different approaches are used to generate the EOS data. One of these approaches is quantum molecular dynamics, which we use to address the high-temperature high-pressure part of the EOS. Here we report our QMD results for the structure, composition and properties of the high-pressure planetary ices. As well as producing usable EOS in their own right, QMD can validate chemical equilibrium calculations, which are based on assumed functional forms for thermodynamic potentials. Where valid, these calculations can be performed much faster than QMD.

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