The winners of the 2007 CAP Best Student Oral Preaentation Competition at the CAP Annual Congress, 2007 June 17-20, in Saskatoon, Saskatchewan were: Isaac Tamblyn (1st), Jonathan Thiessen (2nd), and Francis Torres (3rd). Their extended abstracts are reproduced below. Ed.

INSIDE THE JOVIAN ATMOSPHERE: HYDROGEN AND HELIUM AT EXTREME CONDITIONS

BY ISAAC TAMBLYN, JAN VORBERGER, BURKHARD MILITZER, AND STANIMIR BONEV

SUMMARY

We derive the equation of state of hydrogen and hydrogen-helium mixtures using first principles simulations. These data can be used to refine planetary models.

Since Canadian astronomers discovered the first extra-solar planet in 1988 [1], we now know of almost two hundred and fifty worlds orbiting stars other than our own. While some so-called "Earth-like" planets have been identified, the vast majority of these new planets are gas giants, much closer to Jupiter in character. The discovery of these new planets has challenged existing astrophysical models, and has helped to provide insight into the nature of solar systems, both our own and those of distant stars. Here we report results of first principles molecular dynamics simulations [2,3], based on density functional theory (DFT-GGA [4,5]), of hydrogen and hydrogen-helium mixtures under conditions relevant to gas giants. These data can be used to improve existing planetary models, which depend strongly on the accuracy of input parameters.

One property that is particularly important for the development of planetary models is the equation of state (EOS) of the materials within. An equation of state describes the functional dependence of thermodynamic variables. First principles simulations are useful for determining the EOS of a system, as there are no fitted parameters - the system is governed only by the fundamental laws of physics. Unlike more approximate techniques such as chemical models, properties such as pressure, total energy, dissociation degree, *etc.* are not inputs in first principles simulations but rather are predicted.

In our simulations nuclei are treated as classical particles while electrons are treated quantum mechanically. The ground state electron density is obtained from DFT, from which forces are derived (Born Oppenheimer molecular dynamics). To simulate liquids, we use a supercell of 119 - 128 particles and periodic boundary conditions. The electronic density is expressed with a plane-wave expansion, where the kinetic energy of the highest energy plane-wave is 70 Ry. We use gamma point sampling of the Brillouin zone, and the ionic core is represented with a pseudopotential of the Troullier Martin type [6]. Throughout the simulation, the number of electrons and volume of the simulation cell are held constant, and the ionic temperature is controlled with a Nose-Hover thermostat (NVT ensemble). The stress tensor is monitored throughout the simulations. Typical runs are 1-2 ps in length, ensuring that the system is in equilibrium, and that sufficient statistics can be collected.

In Figure 1, below, we show our calculated equation of state for three systems at the same electronic density, corresponding to $r_s = 1.60$ (r_s is the Wigner-Seitz radius,

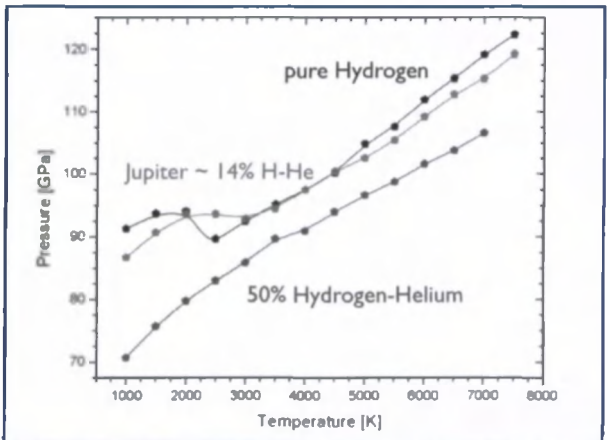

Fig. 1 Equation of state of hydrogen and hydrogen-helium mixtures at an electronic density corresponding to r_s=1.60. The drop in pressure at ~ 2500K occurs as hydrogen molecules dissociate. The magnitude of this drop and the temperature at which it takes place is dependent on the fraction of helium present in the mixture.

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defined as $r_s = \left(\frac{3V}{4\pi N}\right)^{1/3}$). In one simulation, all atoms present are hydrogen. In the remaining two, we simulated hydrogen-helium mixtures at mixing ratios (by mass) of 14% and 50% respectively. The value of 14% was used to approximate the mixing ratio within Jupiter. The 50% and pure case were included in order to determine the effect of helium.

One of the most striking features of the above data is the fact that the pure hydrogen system undergoes a significant drop in pressure for T ~ 2500K. This drop is large enough to result in $\frac{dP}{dT} < 0$. A similar drop occurs in the 14% (Jupiter) mixture, although the magnitude of the drop is reduced, and the temperature range over which it occurs is extended. As we continue to add helium to our mixture while keeping r_s constant, this drop eventually disappears, and the functional form of P(T) approaches that of an ideal gas. During the course of this work, we calculated the EOS for several additional isochors (not shown). These data are qualitatively similar to the case of $r_s = 1.60$, differing only in the nature of the pressure drop. At lower density, the magnitude of the drop is diminished and occurs at higher temperatures. For the lowest density we considered, $r_s = 2.40$, we observed no pressure drop, even in the pure system.

Previous investigations of pure hydrogen [7] have attributed this pressure drop to a phase change in the liquid, characterized by dissociation of molecules and possibly metallization. Our analysis of structural properties such as pair correlation functions and electronic band gap are consistent with these conclusions.

In addition to depending on chemical models for input, a widely used approximation in planetary models is the so-called linear mixing approximation. It assumes that the properties of a mixture, A + B, can be treated as an average of the properties of two pure subsystems, *A* and *B* respectively. This approximation has been used as there is a relatively small amount of data available (theoretical or experimental) on mixtures at conditions relevant to planetary interiors. With our first-principles results for EOS of mixtures it is now possible to test this approximation over a wide range of conditions (Figure 2).

In order for the linear mixing approximation to be exact, the two subsystems must be non-interacting. Considering our results for the EOS of the pure and mixed systems, this approximation is not valid in all regimes. We find that the magnitude of the resulting errors are dependent on the mixing ratio, temperature, and density of the system, and can be greater than 10%. Errors this large can have a significant effect on the predictive power of planetary models and it is therefore our recommendation that the linear mixing approximation be avoided whenever possible.

To understand the physical phenomena responsible for errors in linear mixing, we focus on the region of the EOS that produces the largest error - in the vicinity of the pressure drop discussed previously. We consider the classical probability distribution of each hydrogen atom's nearest neighbour, both for the pure and mixed systems.

This analysis suggests that when helium is added to the pure system (at constant r_s), the molecules within the system become more tightly bound and are less likely to dissociate. Because the intra-molecular potential is stronger, the dissociation temperature is increased relative to that of the pure liquid. Furthermore, the range of temperatures over which dissociation occurs is extended. This results in a smoother transition and is the reason for the variation in linear mixing errors.

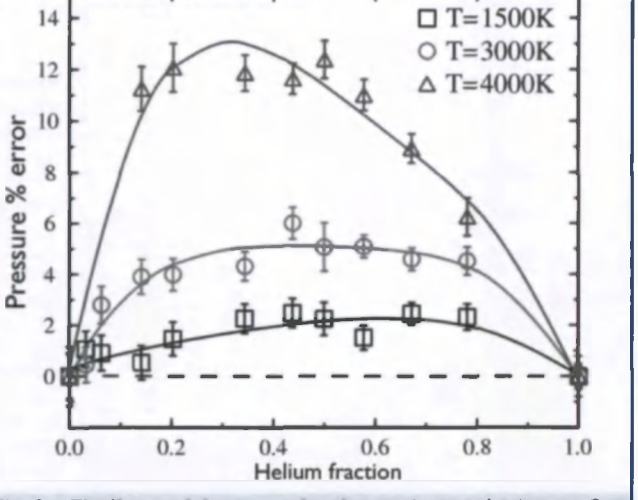

Fig. 2 The linear mixing approximation can be tested using our first principles data. A comparison is made between the pressure predicted from linear mixing (average of pure H and pure He EOS) and what we find in actual simulations of H-He mixtures.

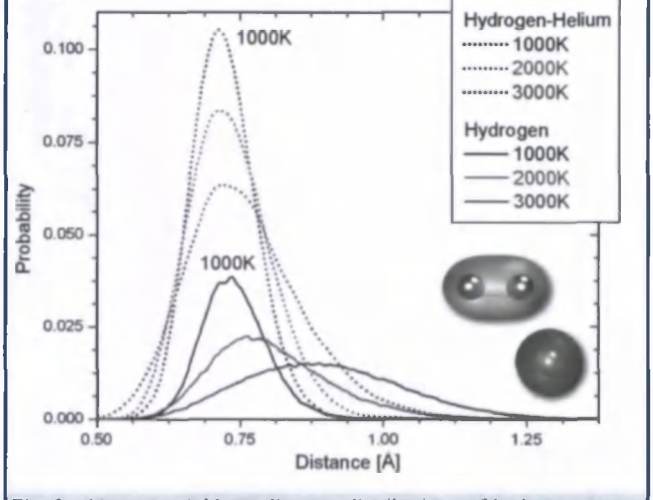

Fig. 3 Nearest neighbour distance distributions of hydrogen atoms for pure and mixed systems at the same electronic density (r_s=1.60). Based on the width of the distributions we see that the presence of helium results in stronger H-H bonds.

We have shown equation of state results from first-principles for pure hydrogen and hydrogen-helium mixtures at conditions relevant to the interiors of gas giant planets. With these new data, we have tested the validity of the widely used linear mixing approximation, demonstrating that it can result in errors on the order of 10%. Furthermore, we have demonstrated that the addition of helium inhibits the dissociation of hydrogen, and thus the nature of the hydrogen EOS.

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