Fluid-fluid phase transition in warm dense matter

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A new idea is introduced that ionization of molecular hydrogen H_2 takes place at the fluid-fluid phase transition in warm dense hydrogen with formation of molecular ions H_2^+ and H_3^+. Conventional ab initio molecular dynamics and quantum simulation techniques are applied for the calculation of the equation of state, proton-proton pair correlation functions g(r) (PCF) and conductivity. The VASP plane-wave code is used. The following results are obtained.
(1) PCF varies slowly with the density at isotherms in the range of distances larger than 2Å. However, the values of the PCF's first local maxima $g(r_{max1})$ and first local minima $g(r_{min1})$ are changed dramatically in a narrow density range. To emphasize the character of g(r) changes, plots of $g(r_{max1})/g(r_{min1})$ are obtained. Strongly pronounced jumps are clear indications of the phase transition since they take place at the same densities where small density jumps are observed. The dependence of discontinuity of ratio $g(r_{max1})/g(r_{min1})$ on temperature gives us the estimation of critical temperature about 4000 K.
(2) The value of r_{max1} is equal to the interatomic distance $d(H_2)$ in the H_2 molecule. The value of r_{min1} is close to the interatomic distances $d(H_2^+)$ and $d(H_3^+)$ in the molecular ions H_2^+ and H_3^+. Let $g_1(r)$ and $g_2(r)$ are PCF's which are the closest to the phase transition before and after it. The function $g(r) = g_2(r) - g_1(r)$ is close to zero for r > 2Å, and has a deep minimum at $r = d(H_2)$ and a strongly pronounced maximum in the range from $d(H_3^+)$ to $d(H_2^+)$. It means that the number of H_2 molecules decreases and a number of molecular ions H_2^+ and H_3^+ appears at the phase transition.
(3) The ratio of the second maxima and minima $g(r_{max2})/g(r_{min2})$ varies smoothly with the density. The PCF's obtained can be modeled by the soft sphere PCF's for r larger than 2Å.
(4) A two-step phase transition mechanism is suggested. The first stage is related to the partial ionization of H_2 molecules with formation of the molecular ions H_2^+. The second stage is the reaction of H_2 molecules and H_2^+ ions to form H_3^+ ions. The phase transition can be related to the Norman-Starostin plasma phase transition prediction. Possible analogs are suggested for substances other than hydrogen.