CHANGES IN PROPERTIES OF H_2 MOLECULES AT THE PHASE TRANSITION IN WARM DENSE HYDROGEN

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The warm dense hydrogen is studied in the region of the fluid-fluid phase transition in the density functional theory framework. A formalized definition of the term "molecule" based on geometry is proposed for calculating the concentration of molecules H_2 and its lifetime. Four relationships are considered.

1. Concentration of H_2 molecules and density along the isotherms. The concentration of molecules is 100% in lower density phase, and smoothly decreases at the phase transition with increasing density.

2. Lifetime of H_2 molecules and density along the isotherms. The lifetime drops sharply by several orders of magnitude during the phase transition. It may be interpreted as ionization of H_2 to H_2^+ since the ions are less stable.

3. Average interatomic distance of H_2 molecules and density along the isotherms. The average interatomic distance has a small but sharp change by 5-8% during the phase transition. It indirectly points to existence of H_2^+ ions as the ions have larger interatomic distance.

4. Concentration of H_2 molecules and conductivity. A sharp increase in conductivity coincides with the onset of the appearance of the ions H_2^+. The increase in conductivity is weak with the further dissociation up to H^+.

This results point to the ionization of H_2 to H_2^+ during the phase transition in warm dense hydrogen. Hydrogen dissociate to atomic molecules with a further increase in pressures (temperatures).

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