

Electron Localization properties across the liquid-liquid phase transition in dense hydrogen.

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We analyze the electronic properties, as characterized by the off-diagonal single electron density matrix and the electron momentum distribution, of high pressure hydrogen across the liquid-liquid phase transition region based on previous Coupled Electron-Ion Monte Carlo calculations [1].

Below the critical temperature the abrupt changes of these distributions indicate a metal to insulator transition occurring together with the structural transition from the atomic to molecular fluid. At higher nuclear temperature above the critical point of the transition, both the change of electronic correlations as well as the change in molecular character of the fluid are continuous. Inspection of electron-proton and electron-electron pair correlation functions provide complementary information of the transition [2,3].

REFERENCES

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