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The role of electrosn in the structure of liquid water MARIA VICTORIA FERNANDEZ-SERRA, University Claude Bernard Lyon-1, EMILIO ARTACHO, University of Cambridge — The structure of liquid water is analyzed by using DFT-based Ab initio molecular dynamic simulations. The essential role that the electronic degrees of freedom play in the the hydrogen bond (HB) interaction is described and a new HB definition based in electrons and not in geometric parameters is proposed. Using this HB probe the structure and dynamics of the HB network in liquid water will be presented, providing new insights interestingly different from the picture that emerges from simulations based on geometrical criteria.

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