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[903] Picture of Wet Electron: A Localized Transient State in Liquid Water

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A transient state of the excess electron in liquid water preceding the development of the solvation shell, the so-called wet electron, has been invoked to explain spectroscopic observations, but its properties have remained elusive. Here, we carry out hybrid functional molecular dynamics to unveil the ultrafast mechanism leading to the hydrated electron. In the pre-hydrated regime, the electron is found to repeatedly switch between a quasi-free electron state and a localized state with a binding energy of 0.26 eV, which we assign to the wet electron. This state self-traps in a region of the liquid which extends up to 4.5 Å and involves a severe disruption of the hydrogen-bond network. Our picture provides an unprecedented view on the wet electron.

Author: Mr PIZZOCHERO, Michele (Chaire de Physique Numérique de la Matière Condensée (C3MP), Ecole Polytechnique Fédérale de Lausanne (EPFL))

Co-authors: Dr AMBROSIO, Francesco (Chaire de Simulation à l'Échelle Atomique (CSEA), Ecole Polytechnique Fédérale de Lausanne (EPFL)); Prof. PASQUARELLO, Alfredo (Chaire de Simulation à l'Échelle Atomique (CSEA), Ecole Polytechnique Fédérale de Lausanne (EPFL))

Presenter: Mr PIZZOCHERO, Michele (Chaire de Physique Numérique de la Matière Condensée (C3MP), Ecole Polytechnique Fédérale de Lausanne (EPFL))

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