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Discovering local order parameters in liquid water using machine learning[1] ADRIAN SOTO, Stony Brook University, DEYU LU, SHINJAE YOO, Brookhaven National Laboratory, MARIVI FERNANDEZ-SERRA, Stony Brook University — The local arrangement of water molecules in liquid phase is still being discussed and questioned. The prevailing view is that water is composed of a mixture of two structurally different liquids. One of the main challenges has been to find order parameters that are able to discriminate the complex structures of these distinct molecular environments. Several local order parameters have been proposed and studied in all sorts of atomistic simulations of liquid water but, to date, none has been able to capture the predicted dual character. This presents an ideal problem to treat with methods capable of unveiling information from complex data. In this talk we will discuss how local order parameters can be constructed from molecular dynamics trajectories by using machine learning and other related techniques.

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Adrian Soto
Stony Brook University

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