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SÉMINAIRE

Mardi 13 décembre, 15h30

*Salle de Conférence, 4ème étage, Tour 22-23, Salle 1
IMPMC, Université P. et M. Curie, 4, Place Jussieu, 75005 Paris*

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WHAT CONSTITUTES A SIMPLE LIQUID?

Simple liquids are traditionally defined as many-body systems of classical particles interacting via radially symmetric pair potentials. We suggest that a simple liquid should be defined instead by the property of having strong correlations between virial and potential energy equilibrium fluctuations in the NVT ensemble. Then, not all atomic liquids are simple and not all simple liquids are atomic. The new definition of a simple liquid shows from computer simulations that a liquid is strongly correlating if and only if its intermolecular interactions may be ignored beyond the first coordination shell (FCS). This is demonstrated by NVT simulations of structure and dynamics of several model liquids with a shifted-forces cutoff placed at the first minimum of the radial distribution function, delimiting the FCS.

The final part of the paper summarizes several properties of strongly correlating liquids, emphasizing that these are simpler than liquids in general. Chemical, physical and mathematical characteristics of simple liquids defined as liquids with strong virial/potential energy correlations are discussed.