Institut de Minéralogie et de Physique des Milieux Condensés
Unité Mixte de Recherche 7590
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SÉMINAIRE
Lundi 18 novembre, 10h30

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

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MOLECULAR DYNAMICS ON COMPOSITION AND MECHANICAL PROPERTIES OF BITUMEN

Bitumen is one of the essential components of roads. Its mechanical properties need to be controlled in order to reduce the rolling resistance between the tyre and the road.
I propose here a bitumen model in order to link molecular composition to mechanical properties of "Cooee" bitumen. This model is composed of four realistic molecule types among which there are large and flat aromatic molecules: asphaltenes. Molecular dynamics (MD) simulations are able to reproduce the aggregation of asphaltene molecules. The size of the nanoaggregates has been estimated and shown to be comparable to experimental results. The dynamics of the nanoaggregates has been precisely quantified. Finally, the influence of these nanoaggregates on mechanical properties and overall dynamics has been investigated.

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