# DFT-MD simulations of mixing properties in warm dense hydrocarbons

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Mixtures of carbon and hydrogen at megabar conditions and at temperatures up to one electron volt can be found in a variety of planets of our solar system like Uranus and Neptune and are believed to feature prominently in extrasolar planets. The microscopic structure, the equation of state, as well as transport and mixing properties of hydrocarbons thus strongly influence the inner structure and evolution of these astrophysical objects. We present results of density-functional molecular dynamics simulations for the structure and equation of state of dense CH. We include the non-ideal entropy of mixing in order to calculate mixing properties of hydrocarbons at such conditions. The results of these simulations explain recent experimental findings showing the demixing of carbon and hydrogen and the formation of nano-diamonds at double shock conditions [1]. In addition, we analyze theoretical capabilities and limitations to predict the inelastic x-ray scattering signal off warm dense hydrocarbons with particular focus on the carbon and diamond part, respectively.

## REFERENCES

[1] D. Kraus et al., *Formation of diamonds in laser-compressed hydrocarbons at planetary interior conditions*, Nature Astronomy **1**, 606 (2017).