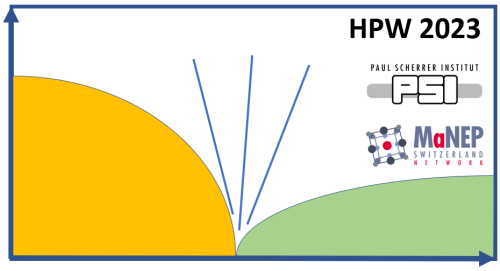

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Molecular dynamics simulations of surface tension of mixtures under high pressures

In this contribution we present theoretical framework for quantitative modeling of surface tension of liquids and their mixtures under high pressures. We perform molecular dynamics (MD) simulations (in GROMACS [1]) and apply statistical thermodynamics of solutions (namely Kirkwood-Buff theory) [2,3]. This allows us to describe solution structure (distribution functions) not only in coexisting liquid phases, but also at the interface, and importantly build its connection to macroscopic thermodynamics (surface tension, chemical potential, etc.).

We will illustrate this framework on MD simulation data of liquid-gas equilibrium of pure methane at a series of subcritical temperatures, presenting surface tension, vapor pressure, and solution structure of coexisting phases.

This methodology is general with respect to number and complexity of components. Thus, once calibrated to experimental data, it will provide atomic insight in novel, industrially relevant, systems studied within the joint GACR-SNSF project "Properties of liquids exposed to pressurized methane, ethane and hydrogen"

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