Abstract Submitted
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Calculating thermal transport coefficients of reverse micelles using molecular dynamics simulations and normal mode analysis HARI PANDEY, DAVID LEITNER, Univ of Nevada - Reno — Ultrafast vibrational studies of reverse micelles reveal that energy transfer from the water inside the reverse micelle to non-polar solvent can be more rapid than energy transfer from the surfactant directly to the solvent [1]. To address computationally the flow of heat in this system, we have calculated thermal transport coefficients for a reverse micelle formed by sodium di-2-ethylhexylsulfosuccinate (AOT) in isooctane over the temperature range 200 K–350K. Because of a "glassy" topology of the reverse micelle we adopted Allen-Feldman theory [2] to calculate thermal transport coefficients, which we have applied to calculate thermal transport coefficients for other soft matter in the past [3]. At room temperature, the thermal conductivity and thermal diffusivity of the reverse micelle was found to be 0.13 W/mK and 5.86 $Å^2$/ps respectively, the former agreeing well with experimental values in polyalphaolefins solvent.

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