Models for Data Validation from Fluctuation Solution Theory

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Fluctuation Solution Theory (FST) provides rigorous connections between molecular correlation functions and derivative thermodynamic properties. Integrals of the correlation functions have been modeled via corresponding states and molecular simulations to yield reliable descriptions of fluid-phase properties for many types of systems and substances. Applications have included liquid densities, gas and solid solubilities, and infinite-dilution partial properties, especially of near-critical systems. The methodology leads to reliable tests of certain property data and of models.

The talk will cover the theoretical and modeling fundamentals; show applications for validating compressed liquid density data, as being incorporated into NIST-TDE, and solid-liquid data; and suggest uses for other property data.