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**Understanding network forming reactions and properties through combining computational and experimental methods**

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Poly(hexahydrotriazine)s (PHTs) represent a class of synthetically tunable and dynamic materials that exhibits broad scope in thermal and mechanical properties. Depending on monomer choice, these thermosets can range from elastomeric and self-healing to strong and brittle. Highly crosslinked thermosetting networks such as these have limited solubility in organic solvents; thus, solid-state analysis was coupled with *in silico* methods to characterize structure-property relationships. Density functional theory (DFT) on small-molecule model systems and molecular dynamics (MD) simulations on network-formation provided a rationale for observed properties and guided ensuing experiments. This talk will focus on the combination of experimental efforts with computational analysis to develop and design new polymeric materials with targeted properties.