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Strategies for design of polymeric nanoparticles JIWU LIU, MICHAEL MACKAY, PHILLIP DUXBURY, Michigan State University — Recently polymer nanoparticles have been synthesized using single chains as macromolecular precursors, providing unprecedented control of nanoparticle size and function. We present the results of molecular dynamics simulations which provide detailed insight into the formation kinetics of specific polymeric nanoparticles and which also predict design strategies for formation of interesting new targets. Nanoparticles are formed through chemical crosslinking which is possible when reactive species on the chain backbone are in close proximity. Since the chemical crosslinking is highly irreversible, nanoparticles formed in this way do not unfold on heating, in contrast to the familiar case of thermal denaturing of proteins. Synthesis of precursors with an alphabet of orthogonal crosslinkers provides a rich phase space for design of polymeric nanoparticles. For example, our simulations indicate that an alphabet of three orthogonal crosslinkers enables self-assembly of two-faced or Janus nanoparticles and a variety of other morphologies.

Phillip Duxbury
Michigan State University

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