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Molecular dynamics studies of entangled polymer chains

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Molecular Dynamics Studies of Entangled Polymer Chains

Monica Bulacu

- Front cover:** Illustration of the entanglement among four polymer chains selected from a dense ensemble of chains, at an arbitrary moment during the molecular-dynamics simulation.
- Back cover:** Surface plot of the combined bending-torsion potential V_{CBT} used in this thesis to control the chain stiffness along the polymer backbone.

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