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Linear Viscoelastic Response of PBX-9501 Binder using Molecular Dynamics Simulations HEMALI DAVANDE, OLEG BORODIN, GRANT SMITH, University of Utah — Quantum-chemistry based force fields for Estane, bis-dinitropropyl formal (BDNPF) and bis dinitropropyl acetal (BDNPA) plasticizer have been developed, validated and utilized in atomistic molecular dynamics (MD) simulations of a model PBX-9501 binder. The viscoelastic response of unentangled binder melt using MD simulations was studied. These results were then used in prediction of linear viscoelastic response of an entangled melt using theoretical models for viscoelastic response of block copolymers and compared with experiments.

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