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Novel Modelling Tool for Energetics LICIA DOSSI, Centre for Defence Chemistry, Cranfield University, Defence Academy of United Kingdom, — Polymer science combines an understanding of chemistry and material properties to design, develop, model and manufacture new materials with special properties for new applications. The *Binders by Design* UK programme, funded through the Weapons Science and Technology Centre (WSTC) by the Defence Science and Technology Laboratory (Dstl), develop new polymeric materials for energetic applications that can survive over the increased operating temperature ranges of future weapon platforms and satisfy international and national regulations. A multidisciplinary team of UK chemists, physicists, modellers and end users (Cranfield University, Sheffield-Hallam University, QinetiQ, Fluid Gravity Engineering, BAE Systems UK Land and Roxel UK) research together on the synthesis, characterisation and modelling of novel macromolecules with very promising thermal properties. Group Interaction Modelling supported by molecular mechanics calculations is used for a rapid assessment and selection of candidate molecules. New model and simulation protocols suitable for investigating the glass transition behaviour of HTPB oligomers are developed. The continuum level models and a constitutive model for a binder/energetic system are developing, for application in safety assessments (e.g. low-velocity impact tests).

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