

POLYMER/PLASTICIZER (HTPB/DOA) BLEND INTERACTIONS WITH A RDX CRYSTAL SURFACE

M. Jaidann ^{1,2}, S. Roy ^{1,3}, H. Abou-Rachid ¹, L.-S. Lussier ¹, J. Brisson ²

¹ *Defence Research and Development of Canada, Valcartier*

² *Chemistry Department, Université Laval, Québec*

³ *Corresponding author's Email: sandra.roy.2@ulaval.ca*

SUMMARY: The interface between a polymer matrix and the various components it contains plays a key role on the resulting properties of the composite. The present work focuses on composite explosive formulations based on crystalline RDX (cyclotrimethylene trinitramine) energetic molecules imbedded in a HTPB (hydroxy-terminated polybutadiene) matrix plasticized using DOA (dioctyl adipate). Results on molecular modelling of this system will be presented. The polymer and crystal are modelled under periodic boundary conditions using the COMPASS atomistic force-field and the Materials Studio software by Accelrys. Molecular dynamics simulations have been performed to study the evolution in time of electrostatic and van der Waals interactions and study the adhesion of the polymer on the RDX crystals, which varies with different atomic (*hkl*) planes. The energy of the polymer-crystal interaction was also estimated.