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The formation of carbon nitride clusters in shocked insensitive explosives¹ LAURENCE FRIED, RIAD MANAA, EVAN REED, NIR GOLDMAN, Lawrence Livermore National Laboratory — Many high explosives are organic molecular crystals that contain both oxidizing and reducing functional groups. These solids rapidly release their energy in supersonic detonation waves. It has been observed that explosives rich in carbon tend to have much longer reaction zones than those that do not. These explosives form graphitic or diamond-like carbon particles during detonation. The slow diffusion-limited process of forming the bulk solid from carbon clusters is believed to play a central role in determining the reaction zone length of a given explosive. In this work, we identify an altogether new mechanism for the slow reactivity of carbon rich explosives. Quantumbased multi-scale simulations of shocked 1,3,5-triamino- 2,4,6-trinitrobenzene (TATB) provide the first evidence for the formation of nitrogen-rich heterocyclic clusters that impede the formation of fluid nitrogen and solid carbon.

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