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Initial reaction mechanisms in crystalline and molten RDX from ab initio molecular dynamics simulations[1] IGOR SCHWEIGERT, U.S. Naval Research Laboratory — Extreme temperatures and pressures are typically thought to have opposing effects on the initial decomposition reactions in energetic molecular crystals: extreme temperatures promote direct bond homolysis (large activation entropies), while extreme pressures should promote concerted reactions (small activation volumes). However, no quantitative data exists regarding the range of temperatures and pressures at which these effects become pronounced. In this presentation, I will describe density functional theory based molecular dynamics simulations aimed at indentifying the mechanism of initial decomposition of crystalline and molten RDX under elevated temperatures (1500 K and above) and pressures (a few GPa and above).

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