Reaction kinetics at extreme conditions

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Nitrated organic compounds combine fuel and oxidizer functionalities within one molecule, react violently in response to even a weak external load, and generate temperatures up to a few thousand K and pressures up to several GPa behind the reaction front. Quantitative kinetic data on the elementary reactions controlling these processes are extremely limited. In this presentation, I will describe an ongoing effort to derive such data for hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) from first-principles molecular dynamics and transition-state theory.

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