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Picosecond timescale detonation of hydrogen azide (HN3)

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Chemical reactions are thought to occur on nanosecond or longer timescales in carbon-containing condensed phase energetic materials. Here we perform the first atomistic simulation of a primary (very sensitive) energetic material, HN3, from the beginning to the end of the chemical evolution and find that the timescale for complete decomposition is only 10 picoseconds, orders of magnitude shorter than that of known materials. This timescale is approaching the fundamental limiting timescale for chemistry, i.e. vibrational timescale. We explore potential deviations of ultrafast detonation from the classical picture where chemistry is slower. The simulations are accomplished using a multi-scale shock simulation method that utilizes the DFTB tight binding method.