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Novel Catalytic Behavior of Dense Hot Water in PETN Decomposition Reactions[1] CHRISTINE WU, LAURENCE FRIED, LIN YANG, NIR GOLDMAN, SORIN BASTEA, Lawrence Livermore National Lab — Under extreme conditions, water is known to exhibit fascinating physical behaviors. Its remarkable structural and phase complexity strongly suggests that its chemical properties may be unusual as well, which have remained largely unrevealed. Using *ab inito* molecular dynamics simulations, we have recently discovered that water plays an unexpected role in catalyzing complex reactions of a high explosive pentaerythritol tetranitrate (PETN). This finding is in contrary to the current view of water as a stable final product of high explosive reactions, and has possible implications in geochemistry, such as reactions in planetary interiors.

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