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Decomposition of energetic molecules by interfacing with a catalytic oxide: opportunities and challenges FENGGONG WANG, ROMAN TSYSHEVSKY, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, USA, ANTON ZVEREV, ANATOLY MITROFANOV, Department of Organic and Physical Chemistry, Kemerovo State University, Kemerovo 650043, Russia, MAIJA KUKLJA, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, USA — Organic-inorganic interfaces provide both intrigues and opportunities for designing systems that possess properties and functionalities inaccessible by each individual component. In particular, mixing with a photocatalyst may significantly affect the adsorption, decomposition, and photoresponse of organic molecules. Here, we choose the formulation of TiO_2 and trinitrotoluene (TNT), a highly catalytic oxide and a prominent explosive, as a prototypical example to explore the interaction at the interface on the photosensitivity of energetic materials. We show that, whether or not a catalytic oxide additive can help molecular decompositions under light illumination depends largely on the band alignment between the oxide surface and the energetic molecule. Furthermore, an oxygen vacancy can lead to the electron density transfer from the surface to the energetic molecules, causing an enhancement of the bonding between molecules and surface and a reduction of the molecular decomposition activation barriers.

Fenggong Wang
Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, USA

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