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Effects of Oxide Surface on the Detonation Initiation of Energetic Materials from First Principles FENGGONG WANG, ROMAN TSY-SHEVSKY, MAIJA KUKLJA, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, USA, UMD TEAM — Organic-inorganic interface provides both intrigues and opportunities for designing systems possessing properties and functionalities inaccessible by individual component. The electronic, catalytic, and defect properties of inorganic surfaces can affect the adsorption, chemical reaction, and photo-responsive properties of organic molecules. In particular, the presence of a particular oxide additive prompts the energy absorption for detonation initiation. Here, we choose the highly catalytic oxide TiO_2 and explosive trinitrotoluene (TNT) as prototypical examples to explore the role of oxide surface on the detonation initiation of explosives from first principles. We show that the TNT- TiO_2 (110) interface induces optical transitions between TiO_2 and TNT, shifting the light absorption edge to lower energy. This helps to control the detonation initiation by laser light with a modest optical energy. In addition, the presence of surface oxygen vacancies leads to electron transfer from surface to molecule, facilitating the decomposition of TNT. Our results not only provide guidelines for designing a controllable oxide-explosive formulation that can be initiated by available lasers, but also help to understand interfaces with target properties and functionalities.

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