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Decomposition Mechanism of Titanium Dioxide (TiO_2) Precursor (Titanium Tetra-Isopropoxide: TTIP) in Flames

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ABSTRACT

Titania (TiO_2) nanoparticles (NPs) have received increasing interest due to their excellent optical properties rendering them promising for a wide range of applications, such as catalysis, medical devices, gas sensing, and solar cells. The performance of those applications are affected by the NP characteristics (e.g., size and morphology), which are significantly controlled by the mechanism by which the particles form.

Flame-made NPs are of great interest due to their fractal-like structures facilitating properties not possessed by their spherical counterparts. Flame synthesis of TiO_2 NPs involves an organometallic precursor being injected into a flame, which subsequently decomposes into $Ti(OH)_4$, followed by nucleation, condensation, aggregation, and agglomeration into fractal-like NPs. Titanium tetra-isopropoxide (TTIP) is one of the most commonly used precursors for the synthesis of TiO_2 NPs in flames, however key steps for the conversion of TTIP into $Ti(OH)_4$ remain poorly studied.

Here, the reaction mechanism of TTIP in flames is revisited using density functional theory (DFT) and a detailed kinetic model. Decomposition of TTIP into the primary intermediate $Ti(OH)(C_3H_7)_3$ is calculated to proceed with a barrier height of 67 kcal/mol, consistent with existing models. We do however identify a novel low-energy decomposition mechanism for the $Ti(OH)(C_3H_7)_3$ intermediate, leading to the production of iso-propanol ($i\text{-}C_3H_7OH$) and C_3H_6 with energy barrier of 37 kcal/mol (Fig.1a). Rate coefficients calculated on the basis of our new mechanism have been used to update the literature kinetic model for TTIP decompostion, and employed to simulate flame synthesis of TiO_2 (Fig. 1b).

By integrating the new decomposition mechanism in each reaction of the Ti-contained intermediate, an upgraded kinetic mechanism for TTIP decomposition into TiO_2 can be developed, matching the experimentally-reported reaction rate constant. Details regarding modifications of existing TTIP decomposition mechanisms, reaction rates, major species, and ignition delay tests will be covered in the talk.

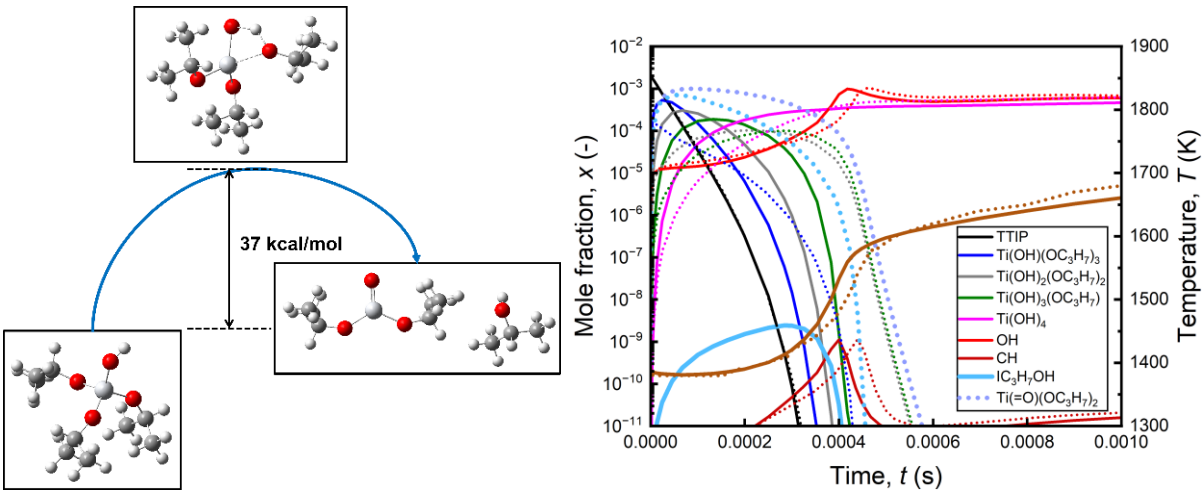

Figure 1: (a) Exampled reaction mechanism of $Ti(OH)(OC_3H_7)_3 \rightarrow Ti(=O)(OC_3H_7)_2 + C_3H_7OH$. (b) Mole fractions of major species. Solid lines are from existing mechanisms, broken lines are after implementating the new mechanism to $Ti(OH)(OC_3H_7)_3$.

KEY WORDS

Titanium dioxide precursor decomposition, hydrolysis, density functional theory, statitical reaction rate theory, photothermal therapy

BIOGRAPHY

Xiaoke Wang is a PhD candidate at The University of Melbourne, Australia. Her research focuses on the fundamental theory of fractal-like nanoparticles on cancer treatment using multiscale simulations of titania (TiO_2) nanoparticles in the gas-phase by molecular dynamics (MD). In addition, she is also interested in exploring the reaction mechanisms of TiO_2 precursors in flames using density functional theory (DFT) and statistical reaction rate theory.

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