

Computational Insights into Crystal Plane Dependence of Thermal Activity of Anion (C and N)-Substituted Titania

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Supporting Information

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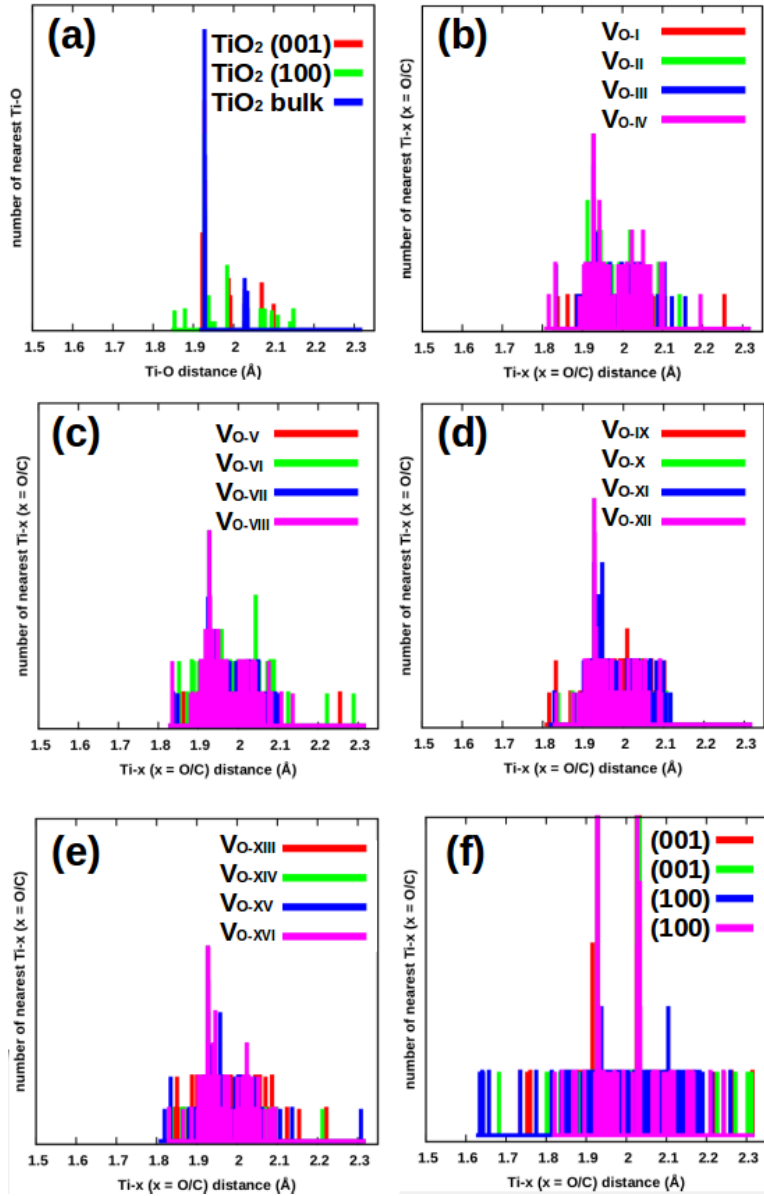


Figure S1: Bond length distribution of (a) surface exposed (001), (100) planes and bulk TiO_2 (b) $\text{V}_{\text{O-I}}$, $\text{V}_{\text{O-II}}$, $\text{V}_{\text{O-III}}$ and $\text{V}_{\text{O-IV}}$ sites (c) $\text{V}_{\text{O-V}}$, $\text{V}_{\text{O-VI}}$, $\text{V}_{\text{O-VII}}$ and $\text{V}_{\text{O-VIII}}$ (d) $\text{V}_{\text{O-IX}}$, $\text{V}_{\text{O-X}}$, $\text{V}_{\text{O-XI}}$ and $\text{V}_{\text{O-XII}}$ (e) $\text{V}_{\text{O-XIII}}$, $\text{V}_{\text{O-XIV}}$, $\text{V}_{\text{O-XV}}$ and $\text{V}_{\text{O-XVI}}$ configurations of $\text{TiO}_{2-2x}\text{C}_x$ bulk and (f) surface exposed (001) and (100) planes of $\text{TiO}_{2-2x}\text{C}_x$.

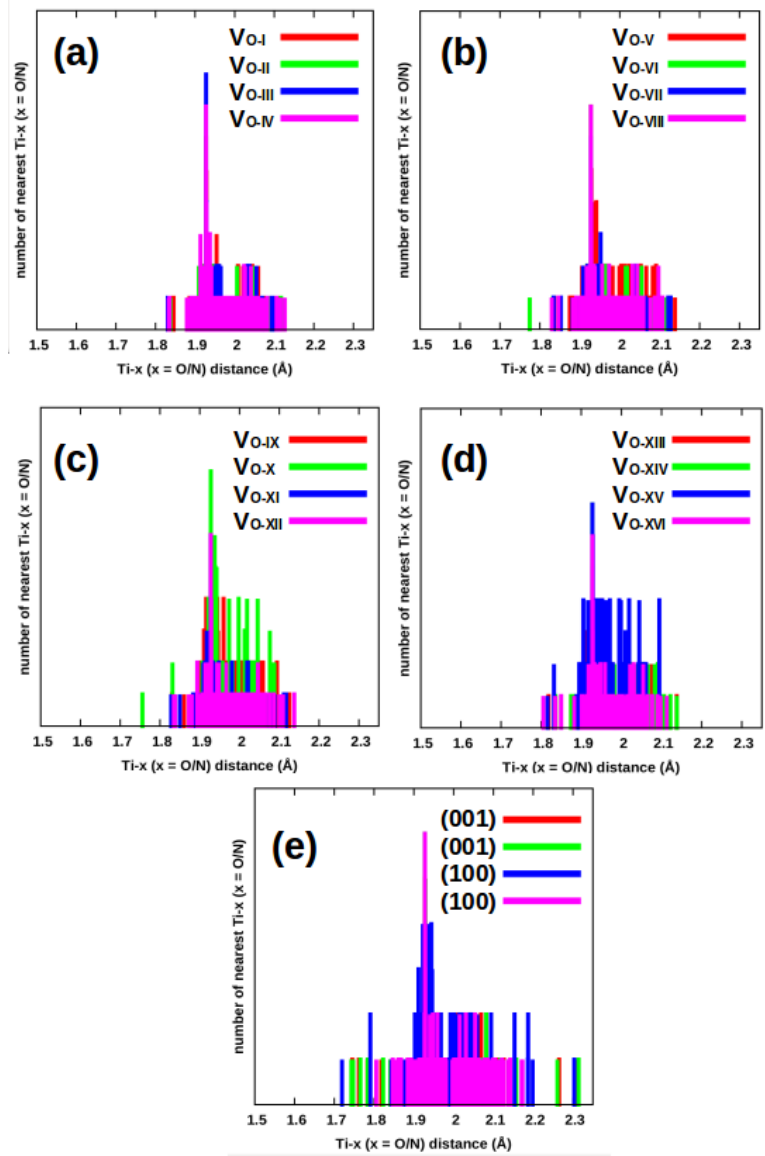


Figure S2: Bond length distribution of (a) V_{O-I} , V_{O-II} , V_{O-III} and V_{O-IV} sites (b) V_{O-V} , V_{O-VI} , V_{O-VII} and V_{O-VIII} (c) V_{O-IX} , V_{O-X} , V_{O-XI} and V_{O-XII} (d) V_{O-XIII} , V_{O-XIV} , V_{O-XV} and V_{O-XVI} configurations of $TiO_{2-3x}N_{2x}$ bulk and (e) surface exposed (001) and (100) planes of $TiO_{2-3x}N_{2x}$.