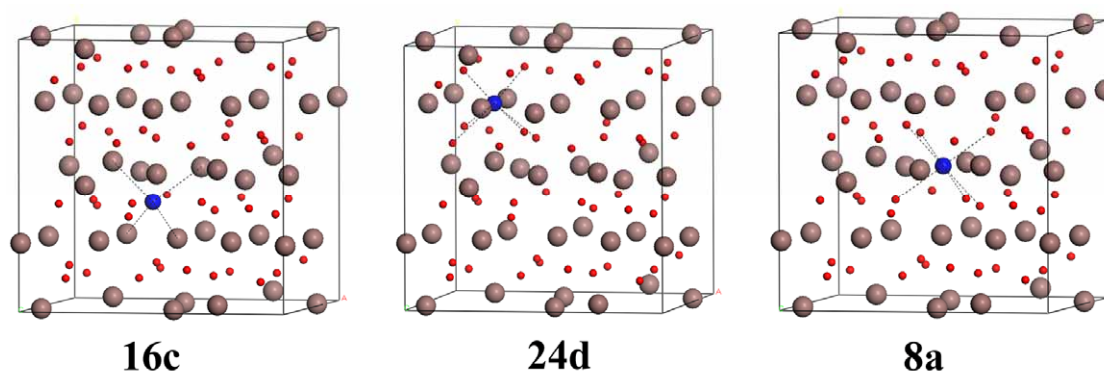


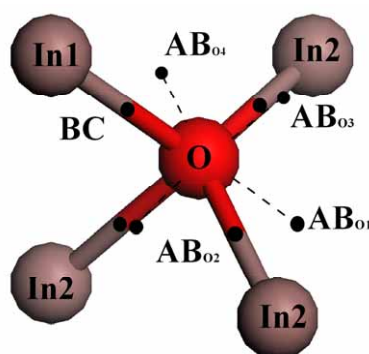
## Supporting Information

### Origin of Improved Visible Photocatalytic Activity of Nitrogen/Hydrogen Codoped Cubic $\text{In}_2\text{O}_3$ : First Principles Calculation

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S1. The original interstitial N positions for 16c ( $1/8, 1/8, 1/8$ ), 24d ( $1/4, 0, 1/4$ ), 8a ( $1/2, 1/2, 0$ ).



S2. The original interstitial N positions for bond center (BC) and anti-bond center (AB) of In-O bonds.