Visible light photoreactivity from Carbon nitride bandgap states in Nb and Ti oxides

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Lamellar niobic and titanic solid acids (HNb$_3$O$_8$, H$_2$Ti$_4$O$_9$) are photocatalysts which can be used for environmental cleanup application and hydrogen production through water splitting. To increase their efficiency, bandgap adjustment which can induce visible light reactivity in addition to ultraviolet light has been one of hot issue in this kinds of photo-catalytic materials. Nitrogen-doping was one of the direction and its microscopic structures are disputed in this decade. In this work, we calculate the layered niobic and titanic solid acids structure and bandgap. Bandgap reduction by carbon nitride absorption are observed computationally. It is originated from localized nitrogen state which is consistent with previous experiments.