Supporting Materials

Improving Visible Light Photocatalytic Activity of NaNbO₃: A DFT based Investigation

Brindaban Modak,¹,² Pampa Modak³ and Swapan K. Ghosh¹,²,⁴*

¹Theoretical Chemistry Section, Bhabha Atomic Research Centre, Mumbai – 400 085, India

²Homi Bhabha National Institute, Mumbai – 400 094, India

³Radiological Safety Division, Atomic Energy Regulatory Board, Mumbai-400094, India

⁴UM-DAE Centre of Excellence in Basic Sciences, Kalina Campus, Mumbai-400098, India

Email: skghosh@barc.gov.in
Phone: 91-22-25595092
Fax: 91-22-25505151
**Fig. S1:** Density of states of (W, N)-codoped NaNbO$_3$ with different ratio of W and N calculated using 2 × 2 × 2 supercell.

**Fig. S2:** Density of states of (W, N)-codoped NaNbO$_3$ with different ratio of W and N calculated using 2 × 2 × 3 supercell.
**Fig. S3**: Density of states of (W, N)-codoped NaNbO$_3$ with different ratio of W and N calculated using 2 × 3 × 3 supercell.