Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Materials

Improving Visible Light Photocatalytic Activity of $NaNbO_3$: A DFT based Investigation

Brindaban Modak,[1,2] Pampa Modak[3] and Swapan K. Ghosh[1,2,4]*

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

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

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

[4]UM-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

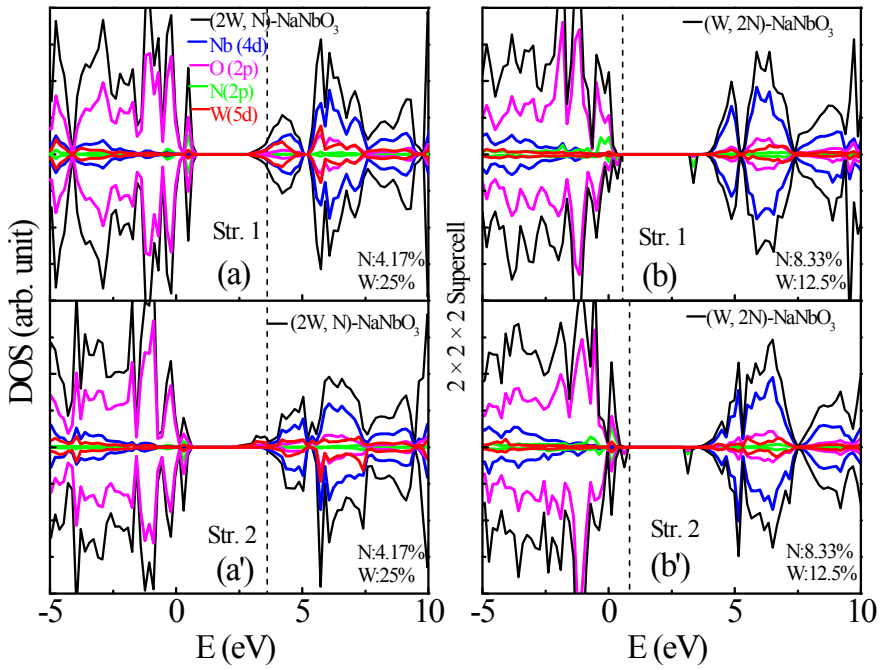

Fig. S1: Density of states of (W, N)-codoped $NaNbO_3$ with different ratio of W and N calculated using 2 × 2 × 2 supercell.

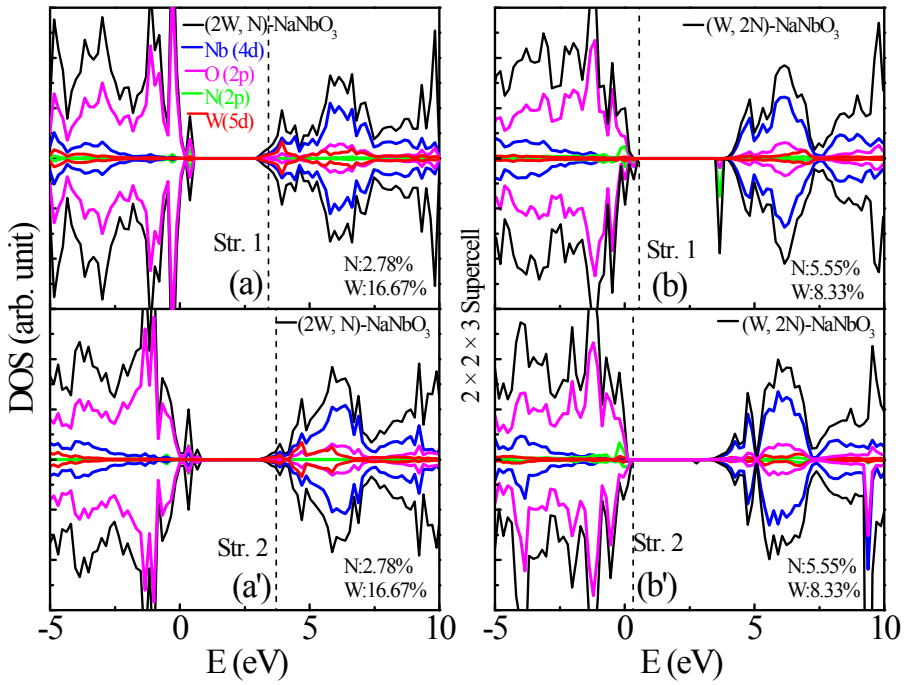

Fig. S2: Density of states of (W, N)-codoped $NaNbO_3$ with different ratio of W and N calculated using 2 × 2 × 3 supercell.

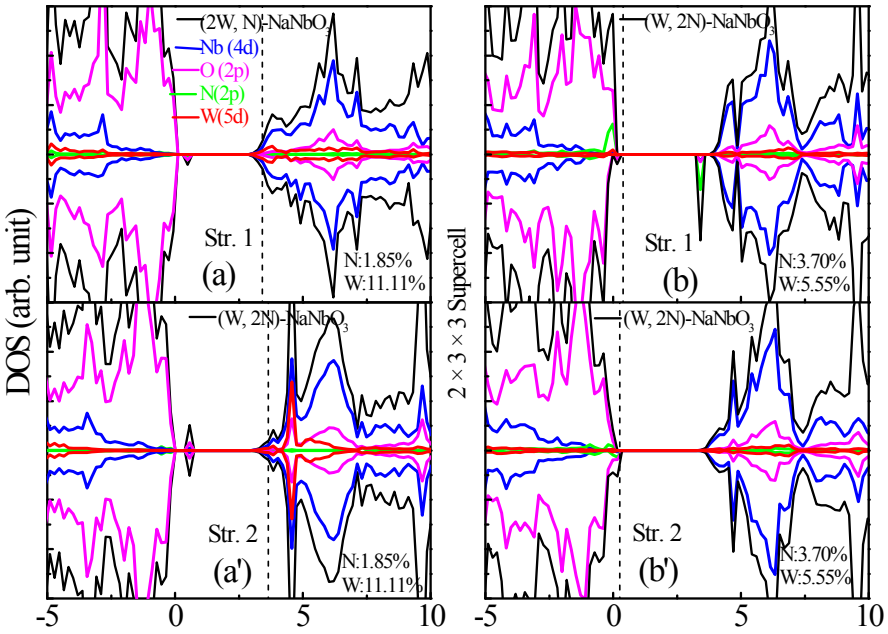

Fig. S3: Density of states of (W, N)-codoped $NaNbO_3$ with different ratio of W and N calculated using 2 × 3 × 3 supercell.