

Local structure of $\text{Bi}_4\text{TaO}_8\text{Cl}$ nanophotocatalyst by npdf analysis

Nalini Ganapathy Sundaram¹, Swetha.S.M Bhat², Mikhail Feygenson³, DiptiKanta Swain⁴, Abhishek Misra⁵

¹Poornaprajna Institute Of Scientific Research, Bangalore 560 055, India, ²Seoul National University, Seoul, seoul, Korea, Rep.,

³Jülich Centre for Neutron Science, Julich, Germany, ⁴SSCU, Indian Institute of Science, Bangalore, India, ⁵Research & Development Department, University of Petroleum and Energy Studies (UPES), Dehradun, India

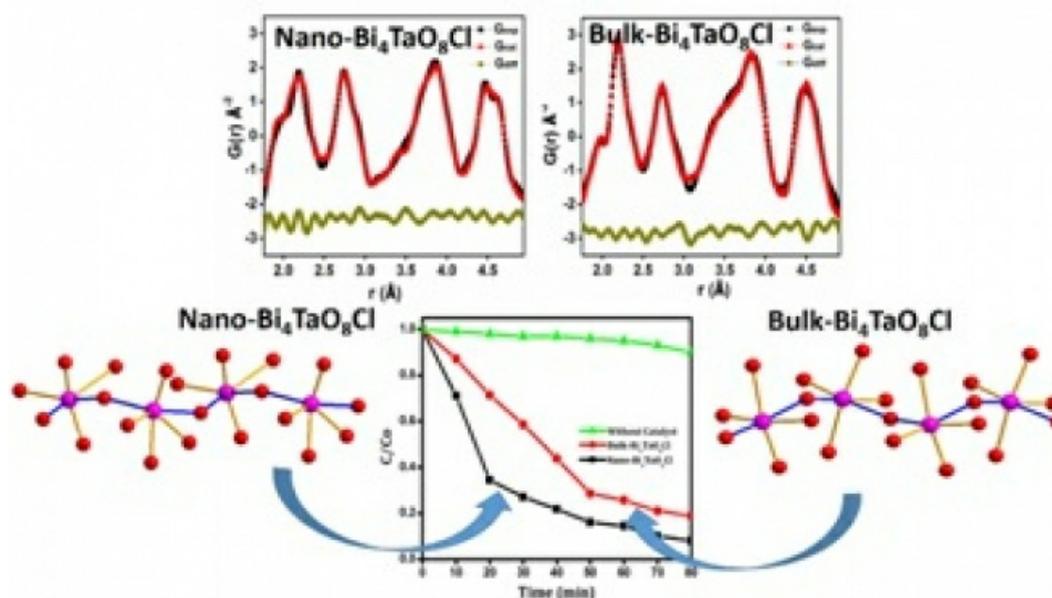
E-mail: nalini@poornaprajna.org

The local structure of Aurivillius-Sillen oxychloride $\text{Bi}_4\text{TaO}_8\text{Cl}$ nanoparticles, studied by neutron pair distribution function (NPDF) analysis, shows a significant local structural deviation of nano- $\text{Bi}_4\text{TaO}_8\text{Cl}$ in contrast to the local structure of bulk- $\text{Bi}_4\text{TaO}_8\text{Cl}$. The PDF of the nanomaterial shows significant homogeneous and inhomogeneous strain. Further, increased distortion of TaO_6 , decreased Ta-O-Ta bond angle and increased octahedral tilt has been established in the local structure of nano- $\text{Bi}_4\text{TaO}_8\text{Cl}$. These structural changes influences the band structure and the electron hole pair migration. The increased octahedral tilt observed in local and average structure affects the band gap of nano- $\text{Bi}_4\text{TaO}_8\text{Cl}$ which was further confirmed by DFT. Specific features in the electronic band structure that indicate lower secondary structural distortions in nano- $\text{Bi}_4\text{TaO}_8\text{Cl}$ has been identified. The PDF analysis is further supported by Raman scattering measurements. Therefore, in addition to morphology and size, local structure of the nanoparticles contributes to the photocatalytic performance. This fundamental understanding of nanomaterials would help in design and fabrication of new efficient photocatalysts for fulfilling energy and environmental demands.

[1] Li, J. et al. (2014), *Nanoscale*, 6, 8473-88.

[2] Ackerman, J.F. (1986) *J. Solid State.Chem.*, 62, 92-104.

[3] Kudo, A. (2000) *J. Phys. Chem. B*, 104, 571.



Keywords: [Aurivillius-Sillen phases](#), [Photocatalysis](#), [Local Structure](#)