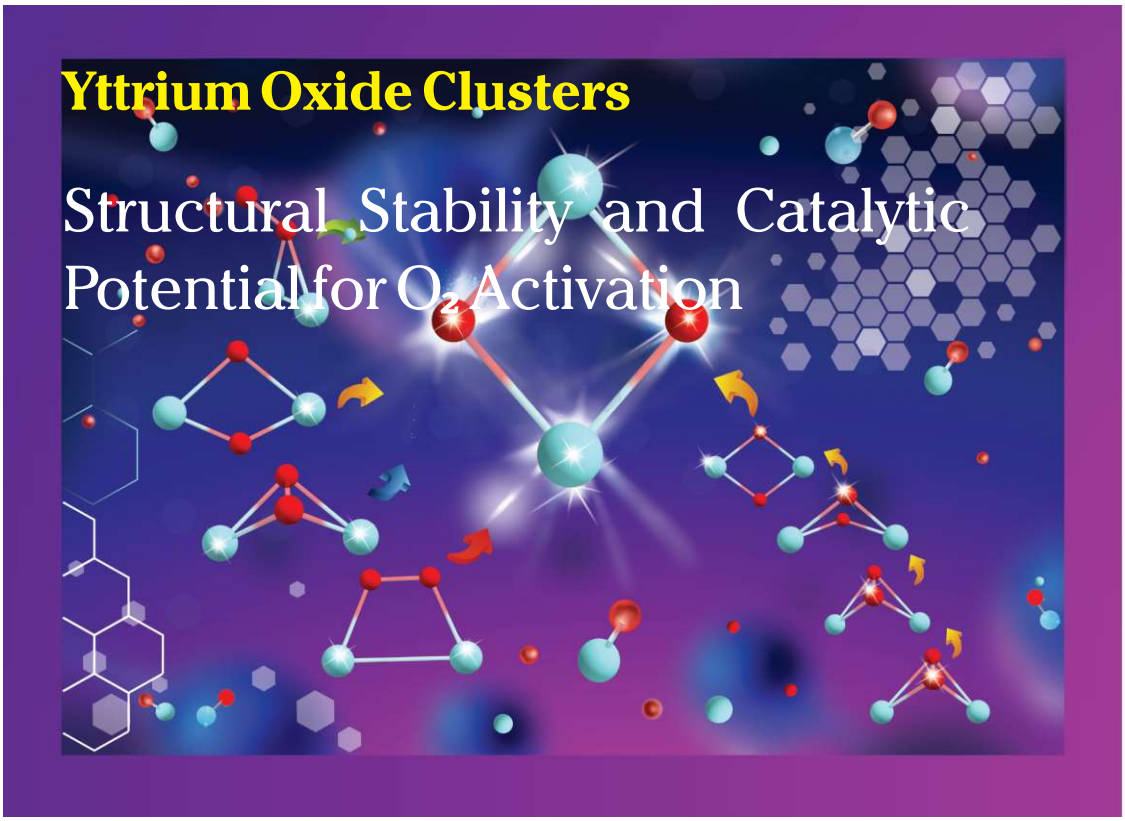

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The study unravels the stable structures of yttrium oxide clusters through threshold photoionization spectroscopy and DFT calculations, revealing stable structures and a newly identified lowest-energy structure for Y_2O_2. These insights position Yn clusters as promising candidates for catalytic O_2 activation.

The figure displayed at the top depicts the ground state structure of Y_2O_2. Several initial structures converged to this and the reaction path after absorbing O_2 on a Y_2 dimer also leads to this stable structure. This figure has been featured as inside back cover of Dalton Trans., 2025, 54, 6402.

This study, conducted at the Atomic and Molecular Physics Division of BARC, explores the structure and reactivity of yttrium oxide clusters (Y_nO_m, where n = 2–8 and m = 2–4), with a focus on their potential to catalyze oxygen (O_2) dissociation. Using threshold photoionization spectroscopy and density functional theory (DFT), the research team investigated the ground-state geometries and ionization energetics of these clusters. For the stoichiometric series Y_nO_2, the authors identified the lowest-energy structures that closely match experimental spectra, including a newly predicted rhombohedral geometry for Y_2O_2. Larger clusters generally exhibit strong structural similarity between neutral and cationic forms, underscoring their resistance to oxidation.

Importantly, the study examines how O_2 interacts with these clusters. While molecular O_2 adsorption is energetically unfavorable, the dissociative adsorption is facilitated at low-coordination sites such as edges and corners. Climbing image nudged elastic band (CI-NEB) calculations reveal that O_2 dissociation proceeds via charge transfer from Y to O, accompanied by significant orbital hybridization. The process leads to the weakening of the O–O bond and formation of stable Y–O configurations, with reaction barriers increasing with cluster size.

Density of states (DOS) and Bader charge analysis further confirm enhanced electron density near the Fermi level, indicating strong Y–O reactivity. These findings position yttrium oxide clusters as promising candidates for O_2 activation and potentially catalytic applications involving oxidation processes. This comprehensive approach provides valuable insights into the design of cluster-based catalysts and advances the understanding of metal oxide reactivity at the nanoscale.

Reference:

Investigating the stable structures of yttrium oxide clusters: Y_n clusters as promising candidates for O_2 dissociation, Varun Vinayak Deshpande, Debashis Bandyopadhyay, Vaibhav Chauhan, Gayatri Kumari and Soumen Bhattacharyya, Dalton Trans., 2025, 54, 6402.