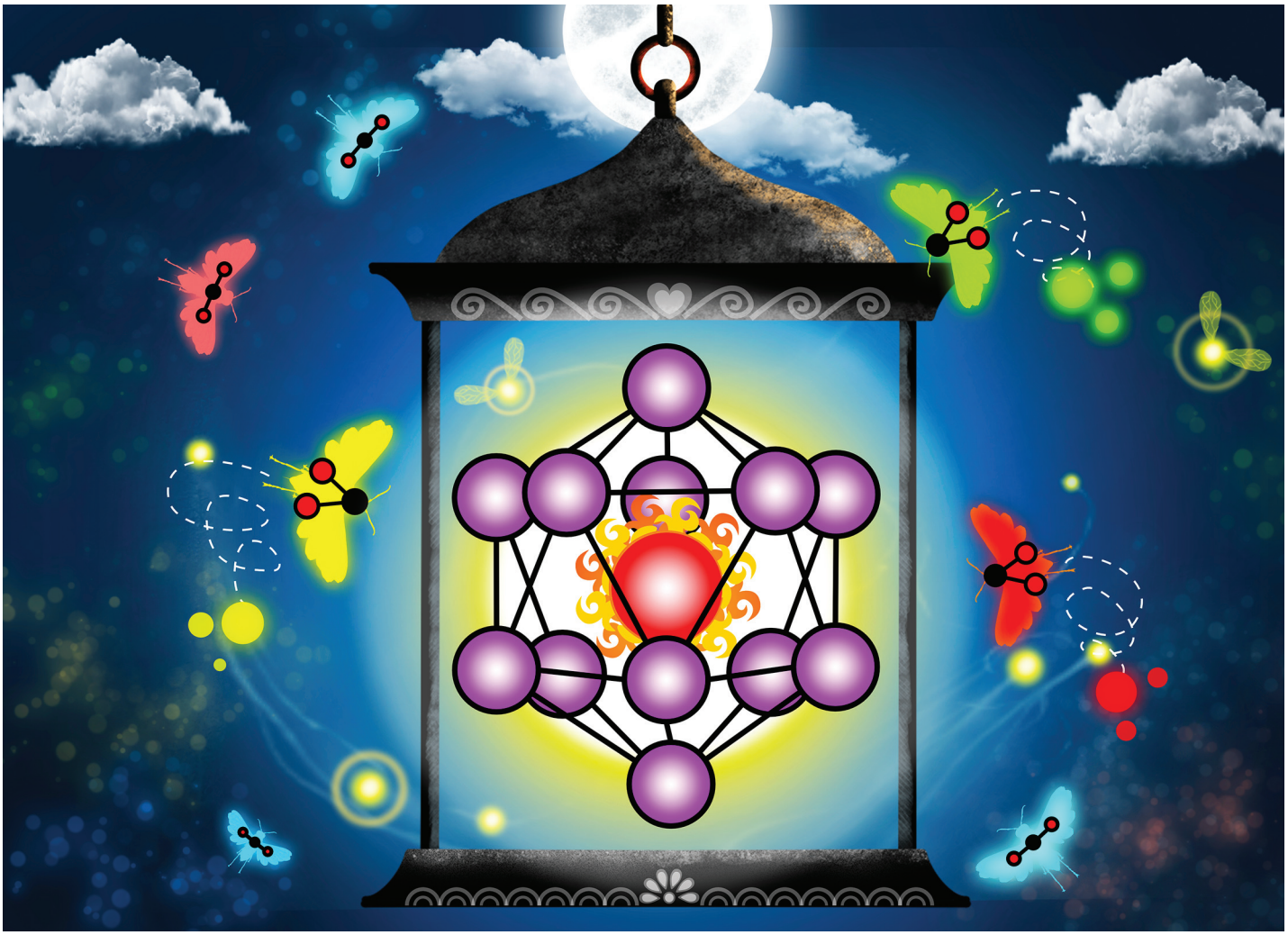

Showcasing research from Professor Puru Jena's group at Physics Department, Virginia Commonwealth University, Richmond, USA.

Activation and electrochemical reduction of carbon dioxide by transition metal atom-doped copper clusters

Transition metal-doped Cu clusters (XCu_{12}, X = 3d/4d elements) significantly enhance CO_2 activation and reduction, addressing Cu's selectivity limitations. Using a multi-scale theoretical approach integrating the Artificial Bee Colony algorithm, extended Tight Binding model, and DFT, stable geometries were determined where X-atoms prefer endohedral positions. These doped clusters exhibit reduced overpotential (~20%) compared to Cu_{13}, offering a promising route to efficient CO_2 electrochemical reduction. An empirical formula derived from DFT data provides further insights, advancing the design of bimetallic catalysts for sustainable chemical conversion.

Image reproduced by permission of Manish Kumar Mohanta from *Nanoscale*, 2025, **17**, 8515.

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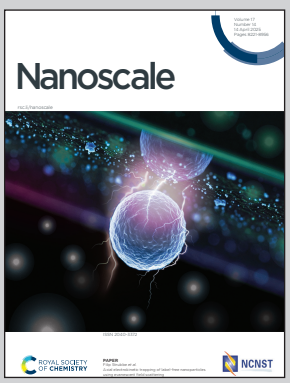

See Manish Kumar Mohanta and Puru Jena, *Nanoscale*, 2025, **17**, 8505.

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