Fine cubic Cu2O nanocrystals serve as highly selective catalyst for propylene oxide production

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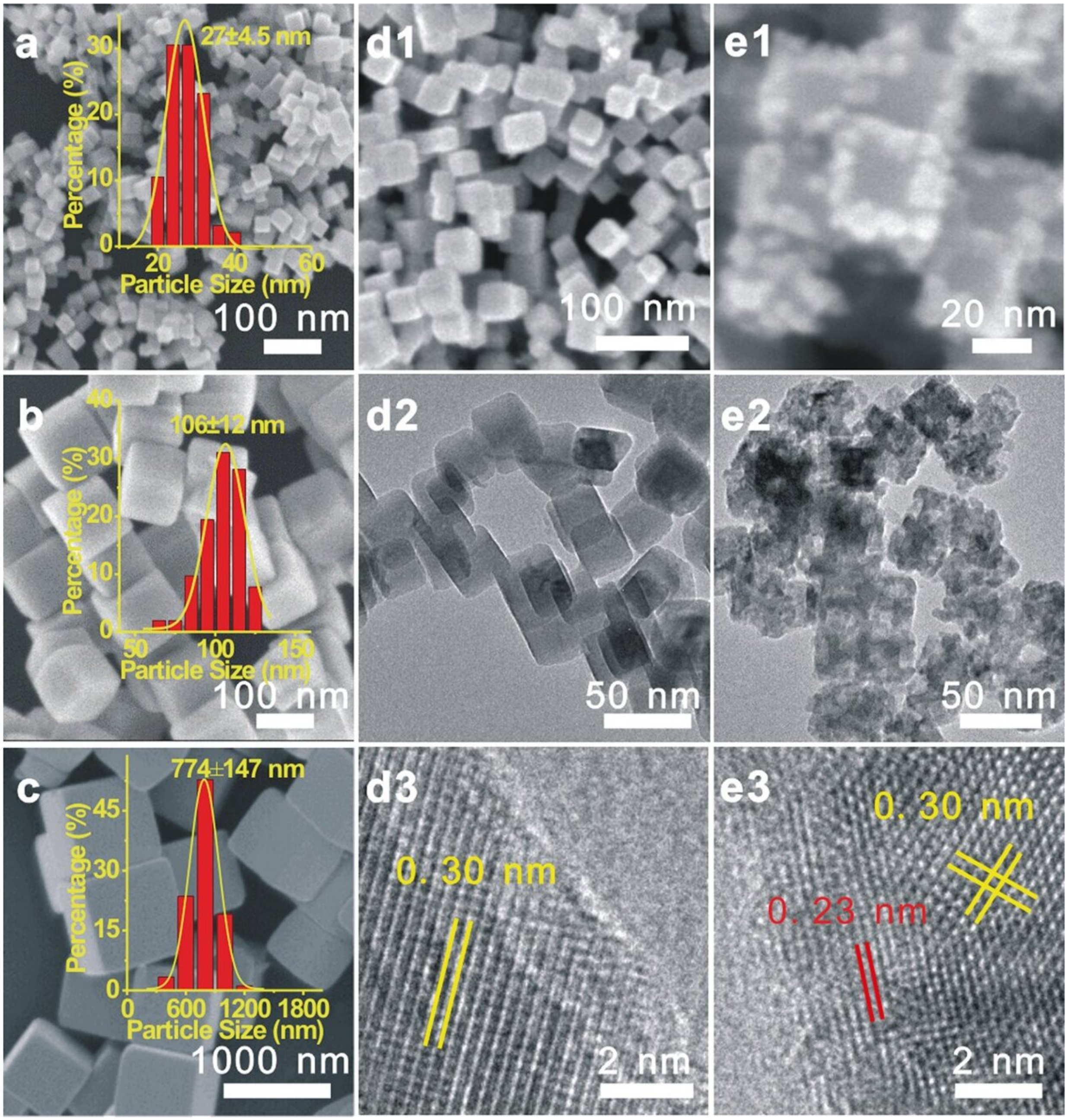

Fig. 1: Microscopic characterization of Cu_2O NCs. SEM images and particle size distributions of a c-Cu_2O-27, b c-Cu_2O-106, and c c-Cu_2O-774. SEM, TEM, and HRTEM images of c-Cu_2O-27 after evaluated in C_3H_6 oxidation with O_2 at 90 (d1–d3) and 150 °C (e1–e3). Lattice fringes of 0.30 and 0.23 nm correspond to the spacing of the Cu_2O\{110\} (JCPDS card no. 78-2076) and CuO\{111\} (JCPDS card no. 89-5899) crystal planes, respectively. Credit: DOI: 10.1038/s41467-021-26257-0

Propylene oxide (PO) is a valuable intermediate product in chemical industry. Current industrial production of PO is neither cost-effective nor environmentally friendly. Propylene epoxidation with O_2 to PO can overcome these drawbacks. However, its practical application is hindered by a lack of efficient catalyst with high selectivity.

The research team led by Prof. Huang Weixin from the University of Science and Technology of China (USTC) of the Chinese Academy of Sciences speculated that Cu_2O\{110\} edges might be crucial in propylene epoxidation reactions based on their previous research on Cu_2O catalysts. However, large rhombic dodecahedral Cu_2O nanoparticles have insufficient \{110\} edges, while Cu_2O cubes finer than 100 nm are much richer in \{110\} edges.

In a study published in *Nature Communications*, Prof. Huang's team constructed fine cubic Cu_2O nanocrystals that enabled high selectivity catalysis for propylene epoxidation, and demonstrated the mechanism that endowed Cu_2O nanocrystal with such enhanced catalytic performance.

Utilizing the size effect, the researchers synthesized Cu_2O cubes with an average size of 27 nm, which showed an outstanding PO selectivity at a relatively low temperature. It was confirmed that the abundant Cu_2O\{110\} site was the active site for PO production.

Further investigations into the catalytic mechanism showed a temperature-dependent behavior for the catalyst. Under low temperatures, the reaction was dominated by Langmuir-Hinshelwood (LH) mechanism, in which weakly adsorbed O_2 species served as active oxygen species. Under high temperatures, Mars-van Krevelen (MvK) mechanism played the major role. CO_2 and acrolein were also formed as by-products, which undermined the PO selectivity of the catalyst.

The development of the catalyst with high PO selectivity in propylene epoxidation offers a new approach to designing efficient catalyst for propylene epoxidation.

More information: Wei Xiong et al, Fine cubic Cu_2O nanocrystals as highly selective catalyst for propylene epoxidation with molecular oxygen, *Nature Communications* (2021). DOI: 10.1038/s41467-021-26257-0

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