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## Video Presntation

# Novel n doped defective ordered mesoporous carbon modified by pd-zn dual-atoms for electrochemical reduction of $co_2$

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he concentration of carbon dioxide (CO<sub>2</sub>) in the atmosphere has exceeded 400 ppm, causing a huge impact on the global environment and economy. The conversion of CO<sub>2</sub> to value-added chemicals (fuel) through electrocatalysis is a hot research direction to address the CO<sub>2</sub> issue. However, the dissociation of carbon dioxide, with carbon-oxygen double bonds in molecules, requires huge energy (about 750 kJ mol-1), which directly leads to an increased cost of conversion with high energy consumption. Therefore, it is of great significance to develop a highly active electrocatalyst to suppress the excessive reduction potential. Compared with bulk metal catalysts, atomic catalysts enable to fully contact with catalytic substances and achieve nearly 100% atomic efficiencies. At atomic scale, the d-orbital of a metal atom in single-atom catalysts (SACs) is close to the Fermi level, which can provide rapid electron transfer and promote the adsorption of CO<sub>2</sub> intermediates. But SACs with only one active metal atom are difficult to break the linear scaling relationships between the adsorption energies of reaction intermediates. In this study, we creatively prepared N doped defective ordered mesoporous carbon (N-CMK-3-D) modified by Pd-Zn dual-atom catalyst for the efficient CO<sub>2</sub> electro-reduction reaction (CO<sub>2</sub>RR). By introducing N atoms into carbon skeleton of CMK-3-D, the lattice structure is deformed and the catalytic properties of the material are improved. Besides, the abundant defects on CMK-3-D does not only act as catalytic active sites but also anchor metal ligands by the 'trapping

effect of defects', which significantly prevent the migration and agglomeration of metal atoms during high-temperature calcination. With modified by Pd-Zn dual-atoms, the catalysts exhibit superior  $CO_2RR$  performances with 97.14% FECO at 0.52 V vs. RHE and an exceptionally high TOF value of 14633 h-1 at -0.72 V vs. RHE with long-term stability, far exceeding that of Pd or Zn SACs. The reason for highly efficient  $CO_2RR$  performance of the catalyst is ascribed to the synergistic effect between Pd-Zn dual-SACs. This novel structure makes the d-band center of metals close to their Fermi level, leading to the change in adsorption energies between metal atoms and  $CO_2$  key intermediates. Thus, the adsorption of COOH\* and the rapid desorption of CO<sup>\*</sup> are enhanced. This work sheds light on a novel design path of electrocatalyts by introducing dual-SACs which exhibit enhanced  $CO_2RR$  electro-catalytic performances by adjusting the electronic structure of the metal active center

#### Biography

Yanlong Gong is a Ph.D. candidate at the College of School of Metallurgy, Northeastern University. He works on structural optimization and performance improvement of electrocatalysts and his current research interests involve the design and synthesis of nanomaterials for electrocatalysis.

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