

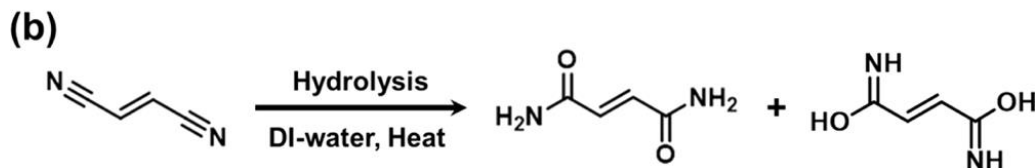
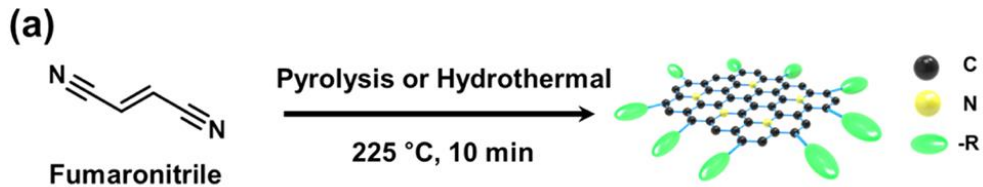
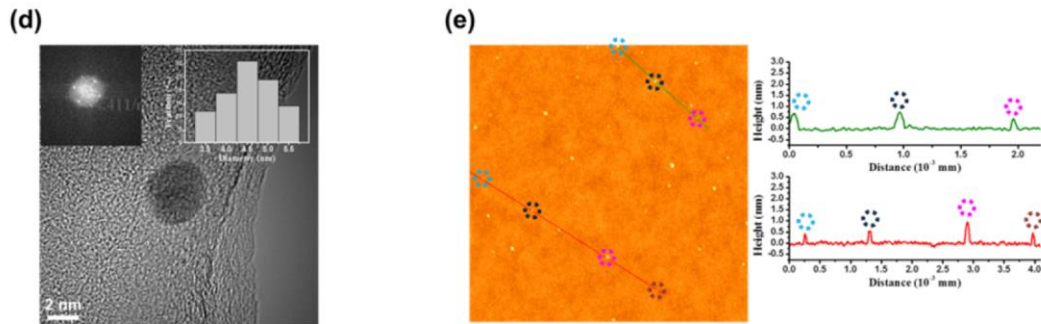
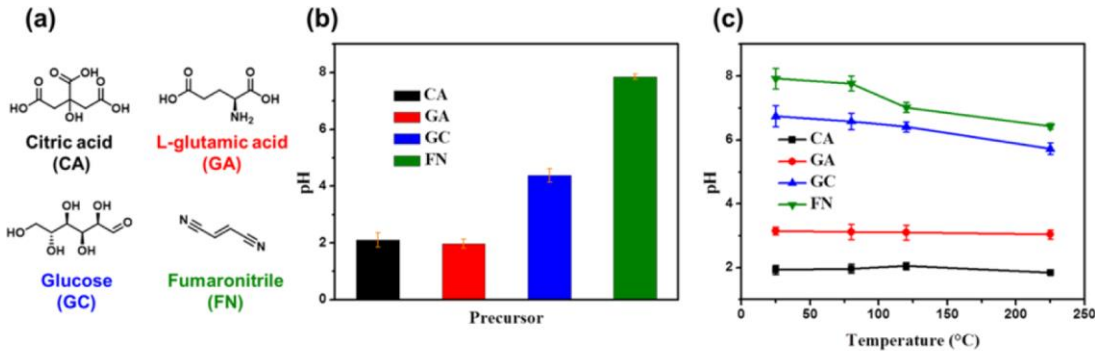
하이드로카본 시스템 효율/안정성 유지 이슈

Efficiency and Stability Issues in Hydrocarbon Reaction System

Uk Sim, Ph. D.

Research of electrochemical CO₂RR

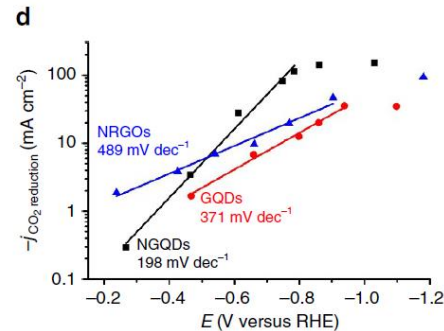
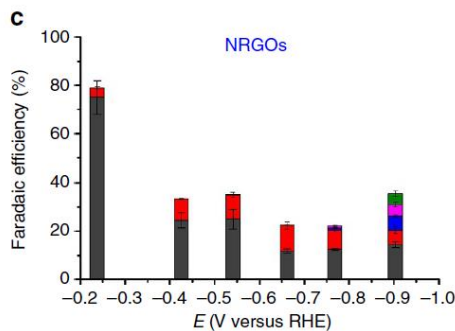
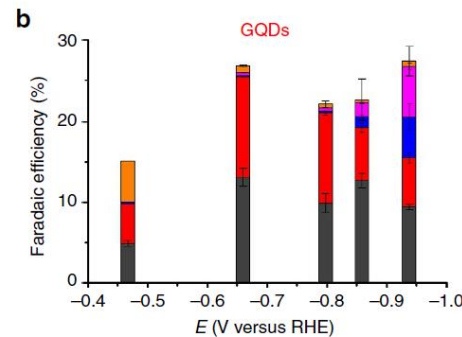
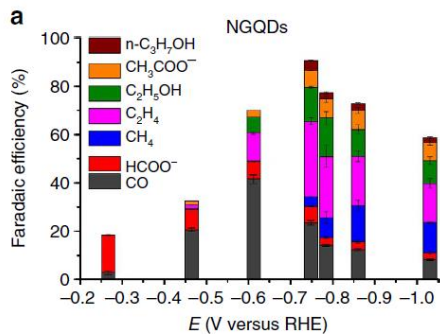
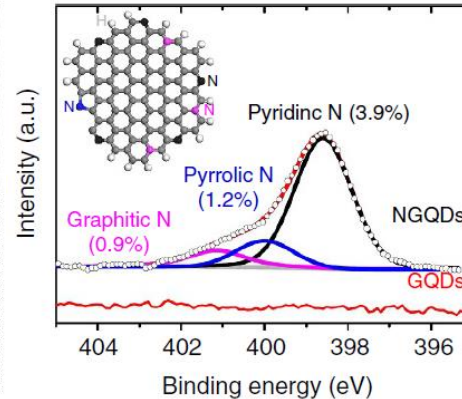
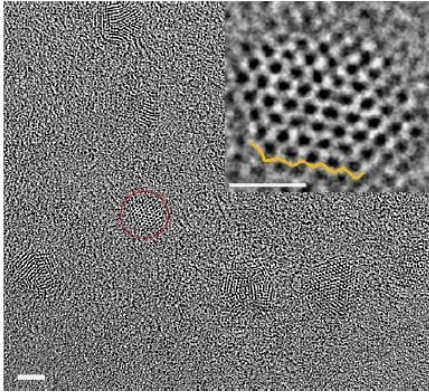
Synthesis and properties of N-CQD



- Facile and eco-friendly synthesis of amphiphilic N-doped graphitic carbon dots with a highly ordered graphitic structure (high sp²/sp³ ratio).
- Excellent stability in various solvents.
- During the pyrolysis, nitrile groups are expected to undergo thermal oxidative degradation and cyclization steps, whereby they become carbonized and finally form relatively hydrophobic NGCDs.
- when using a hydrothermal process, the FN powders are partially converted to either amides or imidic acids in DI water at 225 °C and then form amphiphilic GCDs doped with nitrogen via dehydration and condensation reactions.

Research of electrochemical CO₂RR

Effect of N-CQD on CO₂RR



- The NGQDs show a high total Faradaic efficiency of carbon dioxide reduction of up to 90%, with selectivity for ethylene and ethanol conversions reaching 45%.

- The acidic CO₂ molecule prefers adsorbing onto the Lewis basic pyridinic N group in carbon nanostructures

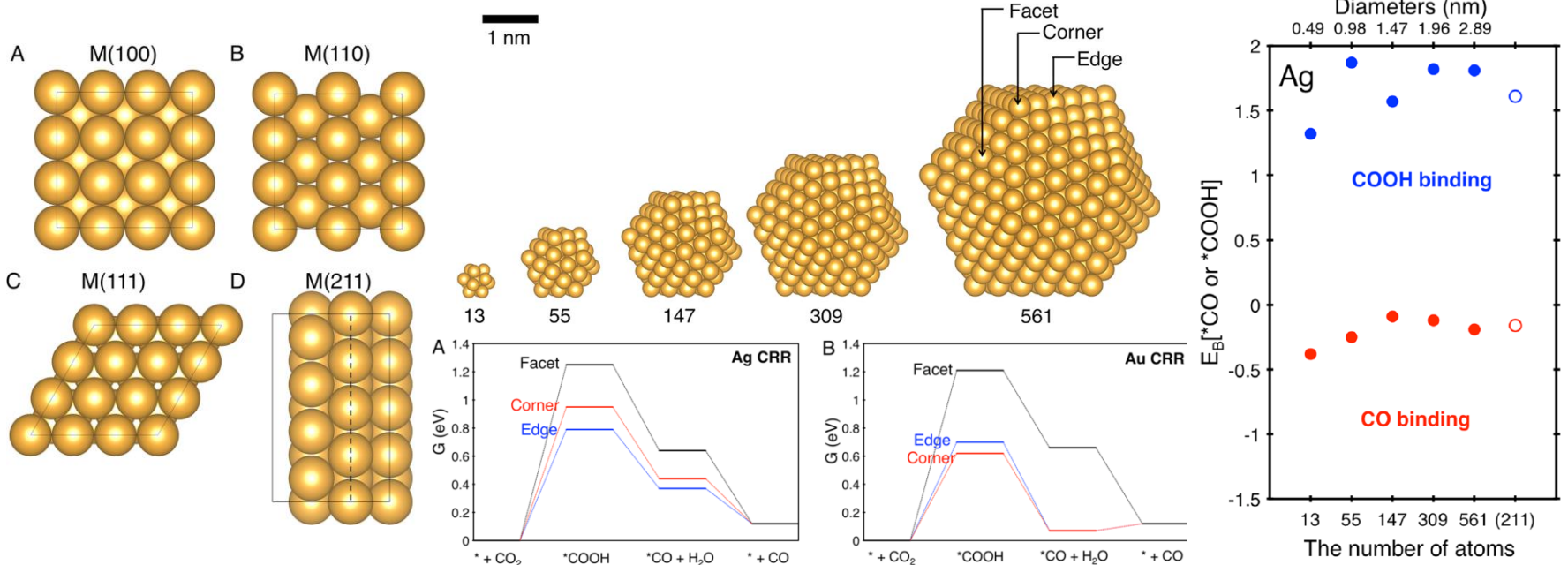
- The pyridinic N at the edge site is believed to be more active to induce C-C bond formation than those at the basal plane, which leads to a higher yield of C₂ and C₃ products on NGQDs electrode than on NRGs electrode.

- The kinetics for CO₂ reduction on NRGs is also slower than that on NGQDs, for example, a Tafel slope of 489mVdec⁻¹ for NRGs versus 198mVdec⁻¹ for NGQDs

Xiaolong Zou et al., ACS Catal. (2017)

Research of electrochemical CO₂RR

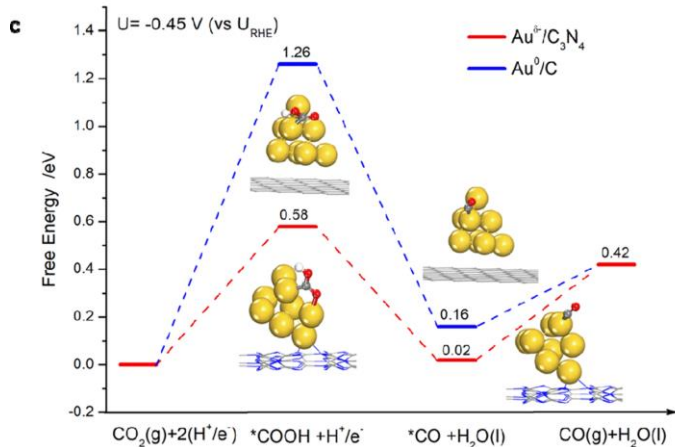
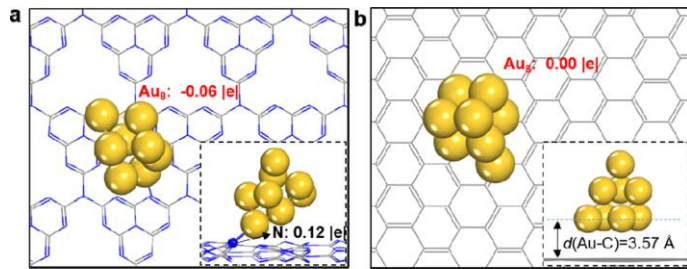
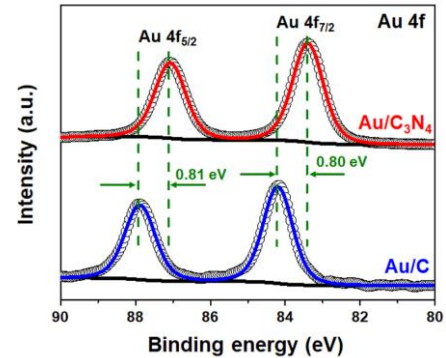
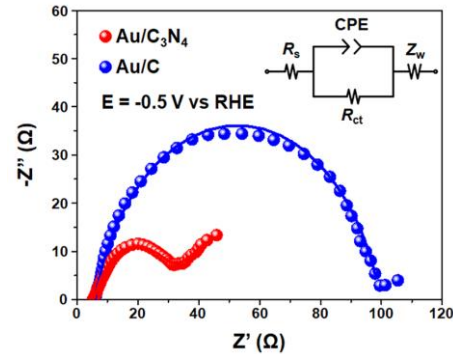
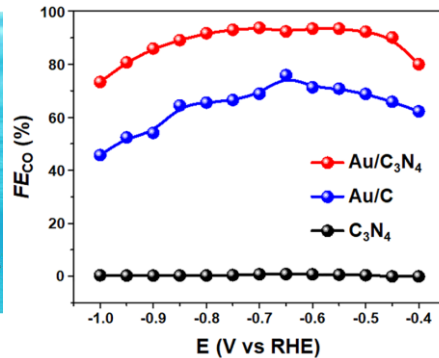
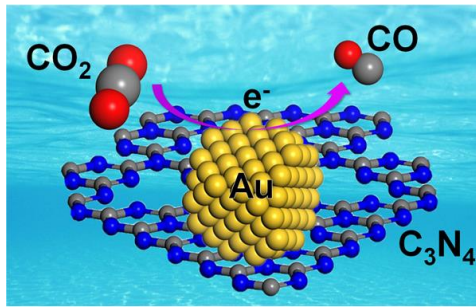
Active Sites of Au and Ag Nanoparticle



- For Ag and Au that bind reaction intermediates weakly at their low-index facets, the under-coordinated sites are the main active sites for the CO₂ reduction reaction.
- In particular, for Au, the corner sites are the main active sites, whereas for Ag, the edge sites are the most active.
- Ag NPs become more active compared to the polycrystalline phase for CO₂RR due to an increase in the number of highly active edge sites.
- Ag nanoparticles are an efficient and inexpensive alternative to Au catalysts for electrochemical CO production from CO₂.

Research of electrochemical CO₂RR

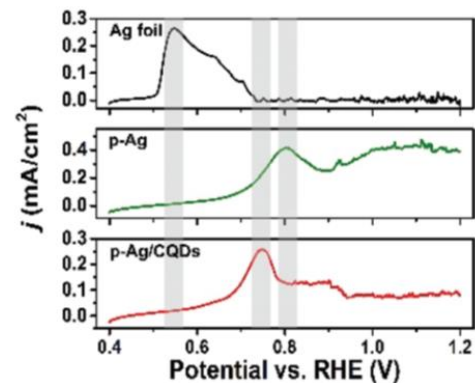
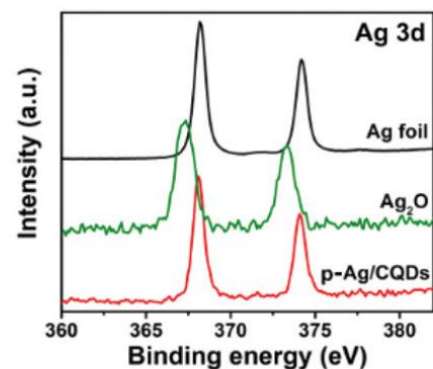
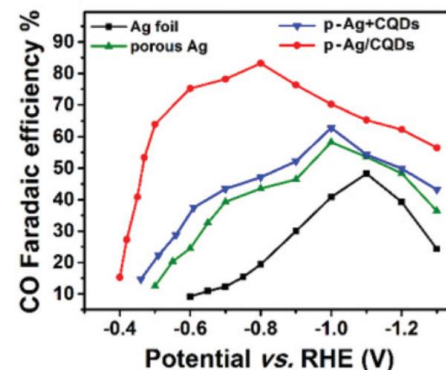
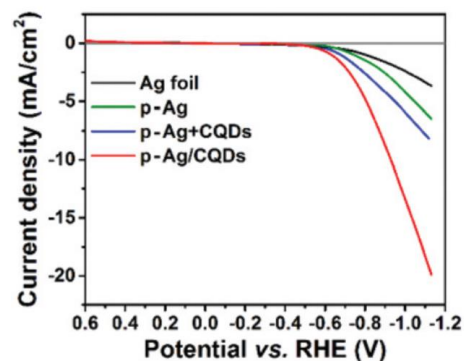
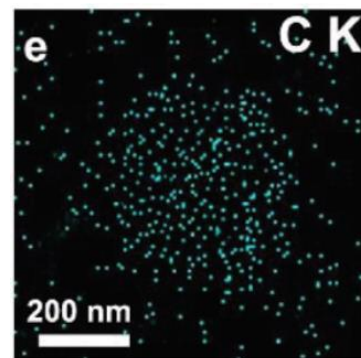
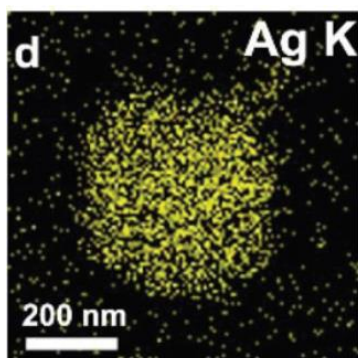
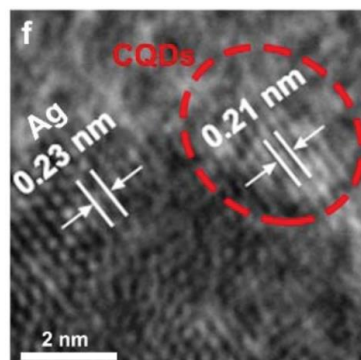
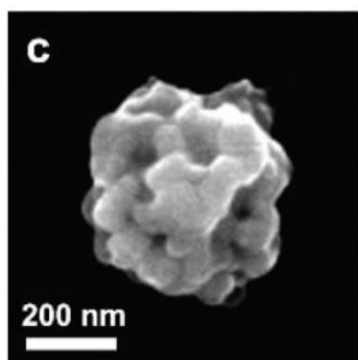
Au/g-C₃N₄



- The fitted R_{ct} of Au/C₃N₄ (19.96 Ω) is much lower than that of Au/C (93.71 Ω), suggesting a faster electron transfer between Au/C₃N₄ and CO₂.
- the Au 4f_{5/2} and Au 4f_{7/2} peaks of Au/C₃N₄ both shift to lower binding energies. Such a shift of binding energy indicates that the Au surface in Au/C₃N₄ is enriched with electrons.
- In comparison with Au⁰/C, one can evidently see that Au^{δ-}/C₃N₄ largely facilitates the electroreduction of CO₂ into *COOH, corresponding to a lower free-energy change of 0.58 eV (vs 1.26 eV for Au⁰/C), rationalized by the improved binding ability of Au^{δ-}/C₃N₄ toward the key *COOH intermediate, relative to Au⁰/C, and thus enhance the CO₂RR.

Research of electrochemical CO₂RR

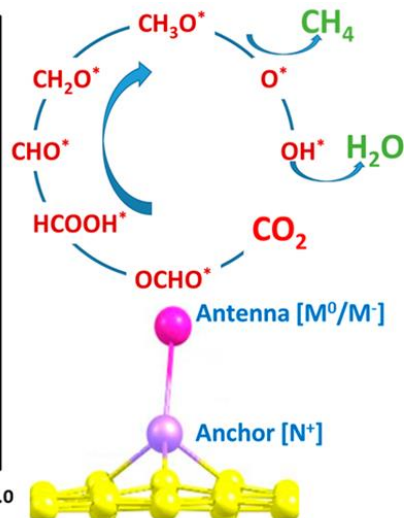
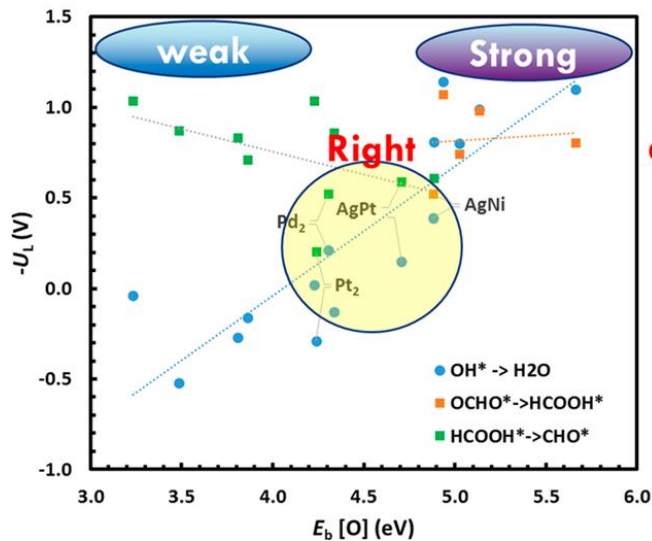
CQD covered porous Ag



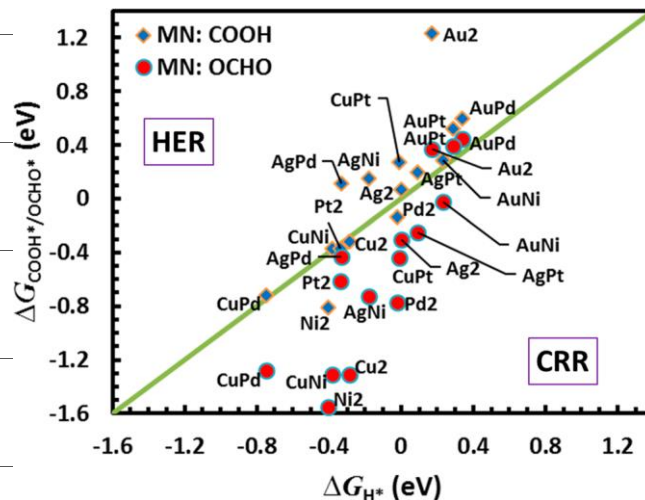
- The positive shift in the peak potential indicates that it is difficult for the CO to be released from the porous structure Ag compared with flat Ag (Ag foil)
- The negative shift in the peak potential and the reduced current density suggest the weaker adsorption of CO on the surface of the p-Ag/CQD composite compared to p-Ag.
- This result indicates that the produced CO is easier to be desorbed from the surface of the p-Ag/CQD composite compared with p-Ag, avoiding the further reduction and promoting the other CO₂ molecules to be reduced.

Research of electrochemical CO₂RR

Graphene-Supported Dimers



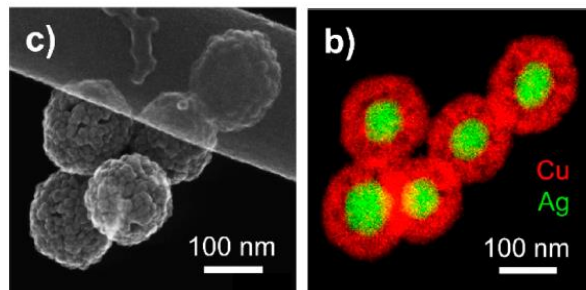
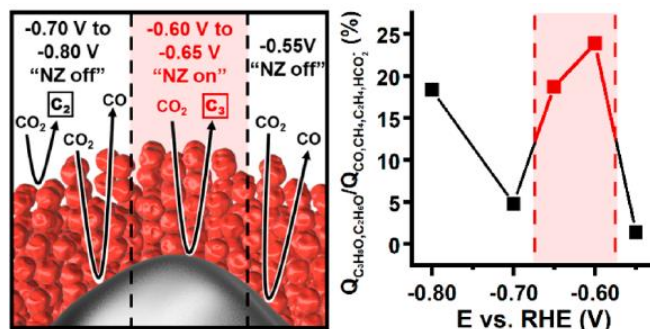
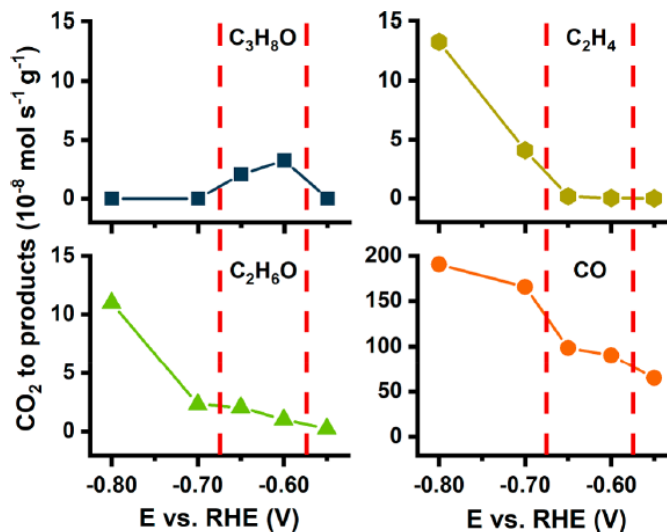
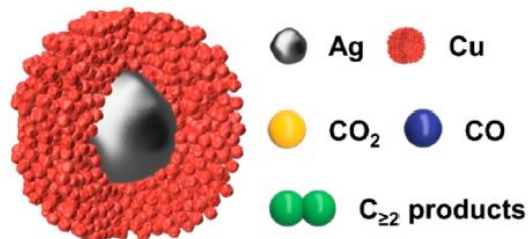
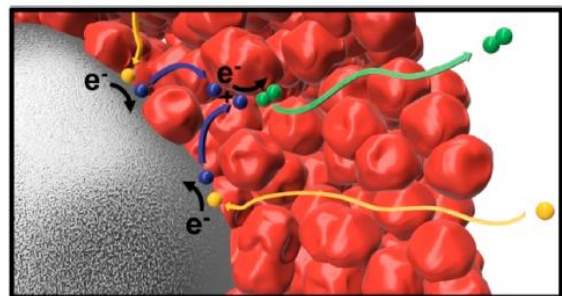
| M ₂ /MN | Ni ₂ | Pd ₂ | Pt ₂ |
|--------------------------|-----------------|-----------------|-----------------|
| E_b [MN] (eV) | 7.23 | 6.98 | 7.90 |
| Q [M] (e), Q [N] (e) | 0.08, 0.45 | -0.02, 0.30 | -0.20, 0.34 |
| R [M-N] (Å) | 2.25 | 2.60 | 2.53 |
| Cu ₂ | CuNi | CuPd | CuPt |
| 3.82 | 6.17 | 5.17 | 6.63 |
| 0.19, 0.47 | 0.12, 0.45 | -0.16, 0.28 | -0.09, 0.20 |
| 2.32 | 2.21 | 2.31 | 2.28 |
| Ag ₂ | AgNi | AgPd | AgPt |
| 2.03 | 6.04 | 5.21 | 6.65 |
| -0.18, 0.33 | -0.14, 0.49 | -0.17, 0.31 | -0.15, 0.25 |
| 2.60 | 2.40 | 2.57 | 2.54 |
| Au ₂ | AuNi | AuPd | AuPt |
| 3.61 | 6.46 | 5.70 | 7.37 |
| -0.30, 0.32 | -0.42, 0.57 | -0.40, 0.40 | -0.33, 0.42 |
| 2.52 | 2.34 | 2.48 | 2.46 |



Haiying He et al., *J. Phys. Chem. C.* (2018)

Research of electrochemical CO₂RR

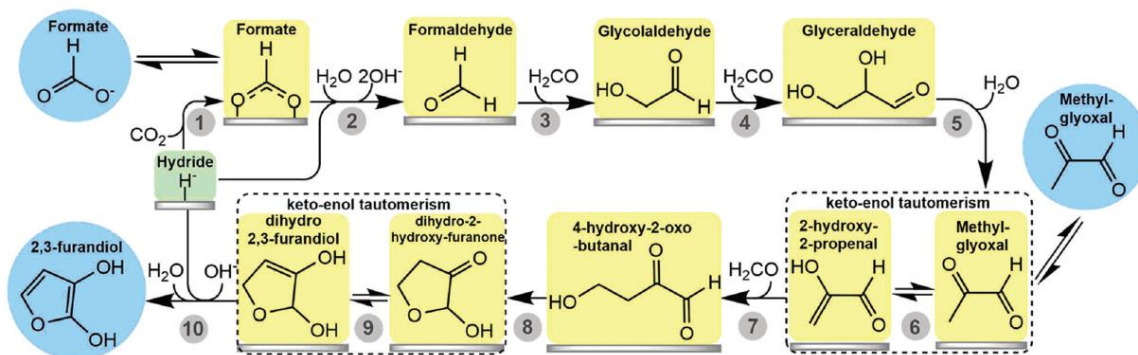
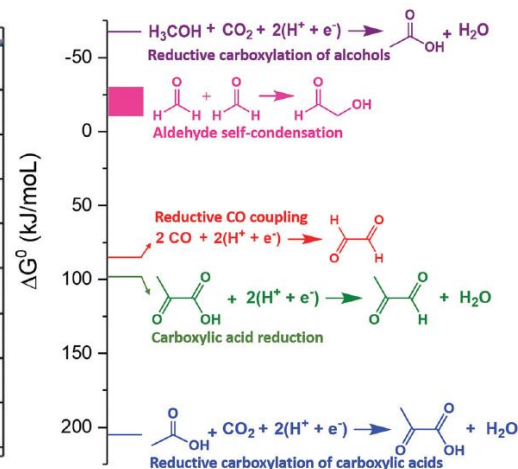
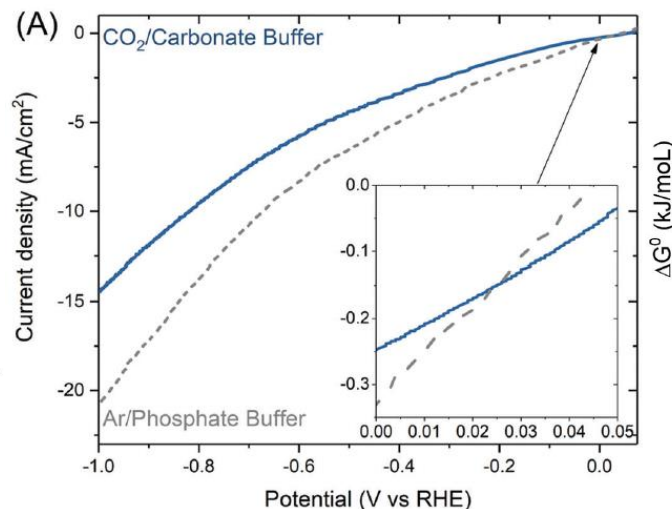
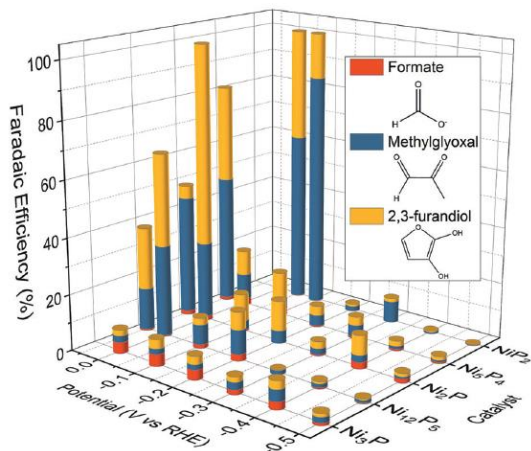
Cascade Reaction in Nanozymes



Peter B. O'Mara et al., *Energy J. Am. Chem. Soc.* (2019)

Research of electrochemical CO₂RR

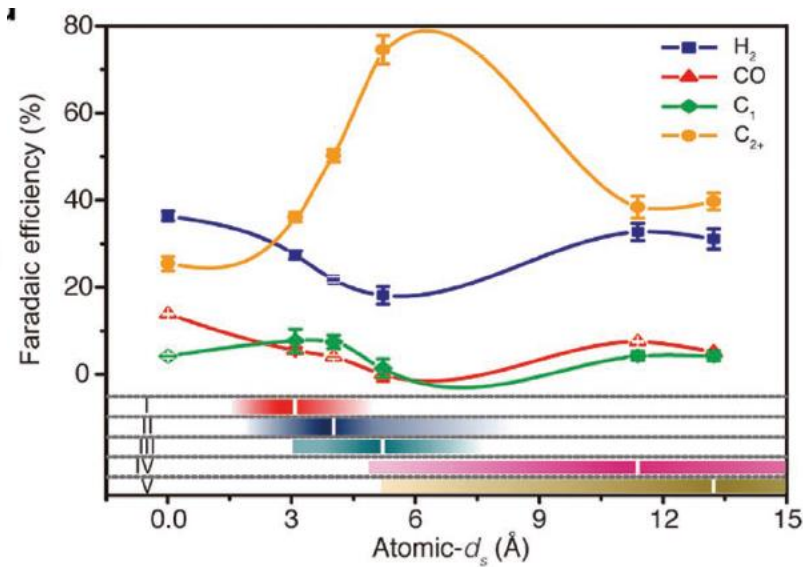
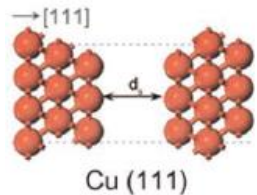
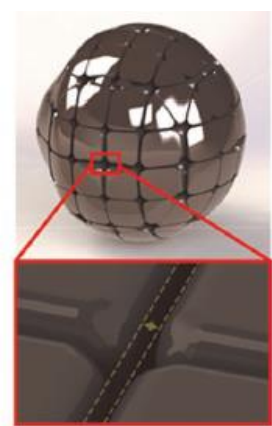
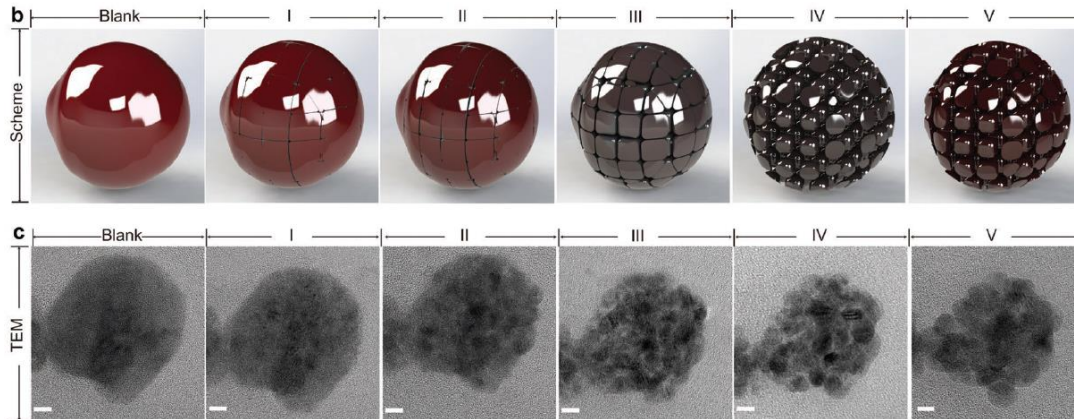
C3 and C4 oxyhydrocarbons on Ni_xP_y



Karin U. D. Calbinho et al., *Energy Environ. Sci.* (2018)

Research of electrochemical CO₂RR

Atomic-Scale Spacing (Defect control)



Hyung Mo Jeong et al., *Adv. Energy Mater.* (2020)