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Literature Seminar

When: April 18, 2024
Time: 1:30 p.m.
Location: CBLL-16

Recent strategies for electrocatalytic C-N bond formation for urea synthesis

Abstract: Urea ($CO(NH_2)_2$) is utilized in nitrogen-based fertilizers for agriculture. Electrocatalytic urea synthesis has gained traction as an alternative technology to the conventional energy-demanding industrial urea synthesis method.[1] However, innovative approaches are required to boost the electrocatalytic C-N coupling process and impede the competing reactions. In this presentation, I will discuss recent electrocatalyst design strategies and the current mechanistic understanding of electrocatalytic C-N coupling. Huang et al. reacted CO_2 and NO in water at monometallic zinc nanobelts for electrocatalytic urea synthesis. Characterization and theoretical simulations demonstrated that the C-N bond formation originated from coupling *CO and *NH_2 intermediates. However, the overall efficiency for urea synthesis was modest with a Faradaic efficiency (F.E) of 11.26% at -0.92 V vs RHE.[2] Zhang et al. proposed an approach to enhance the adsorption of N_2 and CO_2 molecules on the surface of ZnMn-N, Cl electrocatalysts. The authors used Mn to help elongate the N≡N bond to couple with a *CO intermediate to realize C-N coupling in a single step in the electrosynthesis of urea. Limited by the bond activation of N_2, a moderate urea production rate and a F.E of 63.5% at -0.3 V vs RHE was achieved.[3] Zhao et al. utilized a $CuWO_4$ electrocatalyst and NO_3^- as the nitrogen source to synthesize urea. To minimize C-C coupling, the catalyst was designed with alternating bimetallic sites, producing a high F.E of 70% at -0.2 V vs RHE. Mechanistic studies revealed *NO_2 and *CO as the primary intermediates which likely amplified C-N coupling at a low overpotential.[1] Based on the knowledge of this literature review, a perspective on the future of C-N coupling in urea electrosynthesis will be given.

References:

(1) Zhao, Y.; Ding, Y.; Li, W.; Liu, C.; Li, Y.; Zhao, Z.; Shan, Y.; Li, F.; Sun, L.; Li, F. Efficient Urea Electrosynthesis from Carbon Dioxide and Nitrate via Alternating Cu–W Bimetallic C–N Coupling Sites. *Nat. Commun.* **2023**, *14* (1), 4491.

(2) Huang, Y.; Yang, R.; Wang, C.; Meng, N.; Shi, Y.; Yu, Y.; Zhang, B. Direct Electrosynthesis of Urea from Carbon Dioxide and Nitric Oxide. *ACS Energy Lett.* **2022**, *7* (1), 284–291.

(3) Zhang, X.; Zhu, X.; Bo, S.; Chen, C.; Cheng, K.; Zheng, J.; Li, S.; Tu, X.; Chen, W.; Xie, C.; Wei, X.; Wang, D.; Liu, Y.; Chen, P.; Jiang, S. P.; Li, Y.; Liu, Q.; Li, C.; Wang, S. Electrocatalytic Urea Synthesis with 63.5 % Faradaic Efficiency and 100 % N-Selectivity via One-step C−N Coupling. *Angew. Chem. Int. Ed.* **2023**, *62* (33), e202305447.