Contribution ID: **80** Type: **Oral contribution**

2D/Metal-oxide-catalyzed reactions studied in confined space underneath hexagonal boron nitride on Cu(111)

Wednesday, 7 December 2022 09:40 (20 minutes)

Catalysis depends on the availability of active sites and the binding strength of adsorbates to these sites. Recently, catalysis in confined space has been suggested to offer enhanced selectivity and reactivity [1,2], while simultaneously reducing the likelihood of catalyst poisoning or degradation [3]. 2D materials on metal substrates have been extensively studied for fundamental confined catalysis experiments because they can be prepared in a structurally well-defined form and can be characterized in great detail by surface science techniques, providing solid experimental reference data for theoretical studies. However, metal-oxide surfaces are generally more catalytically active than their metal counterparts [4], and only recently has a well-ordered 2D/metal oxide interface been prepared. Our group has synthesized a "Cu2O-like"thin film (˜3-4 Å thick) confined in-between a hexagonal boron nitride (h-BN) overlayer and a Cu(111) substrate via O2 intercalation and oxidation of the Cu substrate. Experimental characterization combined with theoretical simulations unraveled the oxide structure, providing an ideal model system for studies of molecular adsorption and diffusion in confined space. To probe the stability of the heterostructure, we attempted to reduce the confined oxide via H2 intercalation through exposure to varying H2 partial pressures (10-5 to 0.1 mbar) and temperatures (room temperature up to 200 ℃) while simultaneously collecting APXPS data. Following exposure to 0.1 mbar at 200 ℃, we observe a decrease in the O 1s core level intensity for the peaks corresponding to the "Cu2O-like" oxide. Furthermore, a slight shift occurs in the B 1s and N 1s core levels to higher binding energy while the peak shape remains intact, suggesting that H2 was able to intercalate and reduce the surface oxide without destroying the h-BN overlayer. Ultimately, we demonstrate the reversible oxidation of the confined Cu(111) surface beneath h-BN.

1. Fu, Q. & Bao, X. Surface chemistry and catalysis confined under two-dimensional materials. Chem. Soc. Rev. 46, 1842–1874 (2017).
2. Li, H., Xiao, J., Fu, Q. & Bao, X. Confined catalysis under two-dimensional materials. Proc. Natl. Acad. Sci. 114, 5930–5934 (2017).
3. Mahvash, F. et al. Corrosion resistance of monolayer hexagonal boron nitride on copper. Sci. Rep. 7, 42139 (2017).
4. Diebold, U., Li, S.-C. & Schmid, M. Oxide Surface Science. Annu. Rev. Phys. Chem. 61, 129–148 (2010).

if "Other", please specify:

I apply for a travel grant

Yes

Primary author: DIULUS, John Trey (PSI - Paul Scherrer Institut)

Co-authors: Ms DONGFANG, Nanchen (University of Zurich); Mr COMINI, Nicolo' (University of Zurich); Prof. IANNUZZI, Marcella (University of Zurich); OSTERWALDER, Juerg (University of Zuerich); NOVOTNY, Zbynek (PSI - Paul Scherrer Institut)

Presenter: DIULUS, John Trey (PSI - Paul Scherrer Institut)

Track Classification: Surface science/chemistry