Contribution ID: **90** Type: **Oral contribution**

Uncovering role of active sites in NO decomposition reaction of nitrogen-doped graphene using simultaneous APXPS and IRRAS

Wednesday 7 December 2022 17:20 (20 minutes)

Noxious NO gas is a harmful environmental pollutant and toxic to many life forms, however as it stands, prominent reactions such as combustion reactions taking place in engines, generate NO by-products and require removal from the exhaust gas to prevent unnecessary exposure. Current technology lacks a sufficient catalyst to effectively breakdown the kinetically hindered NO molecule without interaction of a reducing agent, i.e. NH3, urea, hydrocarbon, or expending a surplus of energy. The advent of new catalyst materials diverging from a traditional metal and metal oxide may prove advantageous, as is the case for perovskite materials, and more ecologically friendly options that have the ability to perform metal-free catalysis. One such promising candidate is nitrogen-doped graphene (N-Gr). Despite numerous studies of N-Gr examining adsorption properties and reaction chemistry, a fundamental understanding of the role of the active sites in the NO decomposition reaction is currently not well understood. We explored the role of two primary active sites (graphitic N, pyridinic N) in N-Gr films composed of 1) purely graphitic N and 2) a mixture of graphitic N and pyridinic N sites. We tracked the electronic and vibrational profiles of reaction intermediates and products using simultaneous in situ ambient pressure X-ray photoemission spectroscopy (APXPS) and infrared reflection-absorption spectroscopy (IRRAS), respectively. We found that the incorporation of pyridinic N sites lowers the temperature of intermediate formation and potentially promotes different reaction intermediates due to different bonding environments between pyridinic N and graphitic N sites leading to higher reactivity.

if ”Other”, please specify:

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No

Author: EADS, Calley (MAX IV Laboratory)

Co-authors: MALANDRA, Gabriel; KNUDSEN, Jan (Lund University); SCARDAMAGLIA, Mattia (MAX IV Laboratory); TEMPERTON, Robert (MAX IV Laboratory); BOIX DE LA CRUZ, Virginia (Lund University)

Presenter: EADS, Calley (MAX IV Laboratory)

Track Classification: Catalysis