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Using APXPS to follow reactions above and below graphene

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Graphene's popularity has boomed since its isolation in 2004 [1]. We can find graphene in multiple domains of modern technology, from sensing and catalysis to functional materials, electronic devices, and energy-related technologies. However, most of these studies lack the characterization of such systems under realistic conditions. With this contribution, we present two recently published studies [2, 3] highlighting the necessity of APXPS studies for implementing 2D materials in modern technology.

First, we address the stability of hydrogen functionalized graphene under mbar pressures [2]. Hydrogen adsorption on graphene is widely used to open a bandgap on the graphene electronic structure, which has clear advantages for its implementation in electronic devices [4]. However, until now, no studies have addressed their stability under mbar pressures. Our study shows that H-dimers motifs on a graphene surface are selectively removed by room temperature oxygen exposure. Interestingly, DFT calculations indicate that the dimer configuration can attack the O=O double bond already at room temperature leading to water or H₂O₂ formation. Moreover, these results present a new and exciting role for graphene in catalysis studies: as an adsorption template for studying how configurational placement of reactants is linked to catalytic function.

The second part addresses the lack of knowledge on the kinetics of confined reactions under 2D materials [3]. Enhanced activity or selectivity of catalyst materials placed in confined environments has already been studied for a variety of systems [5]. However, until recently, most studies focused on ex-situ characterization or studies under steady-state conditions. Our work demonstrates how we can use short pulses of changing gas composition to repeatedly intercalate and de-intercalate molecules into the space between graphene flakes and their metal substrate. In more detail, we study CO and H₂ oxidation below iridium-supported graphene flakes. We show that hydrogen rapidly mixes into the oxygen structure below the graphene and converts it into a mixed OH-H₂O phase. In contrast, we find that CO exposure only leads to oxygen removal and little CO intercalation. Finally, we demonstrate how H₂ mixed into CO can be used as an intercalation promoter to change the undercover chemistry. Our work is a clear example of how APXPS provides a detailed kinetic perspective on the intercalation process and the undercover reaction not accessible until now.

Altogether, we hope our studies will inspire future APXPS catalysis studies of reactions above and below 2D materials.

[1] Science 306, 5696, 666-669 (2004)

[2] J. Phys. Chem. C 126, 33, 14116–14124 (2022)

[3] ACS Catal. 12, 16, 9897–9907 (2022)

[4] J. Vac. Sci. Technol. A 36, 05G401 (2018)

[5] Chem. Soc. Rev., 46, 1842-1874 (2017)

if "Other", please specify:

I apply for a travel grant

Yes

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