Tweaking Atomic Layer Interfaces for Heterogeneous Catalysis to Energy Storage

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Our past research on atomic layer (2D) interfaces has shown that their interfaces play a seminal role in catalysis (photo/electro) while the pristine layers are inert towards the respective process.[1-4] Interfacing of 2D layers seems to be an effective method in developing atomic layers based next generation catalysts which are scalable and reproducible. This addresses one of the lacunas of doped atomic layers based catalysts, where though they are effective,[5] their controllable reproduction is in question due to the variations in the resultant structures with the differences in the synthesis conditions.[6] The interlayer rotation is found to be insignificant in the catalytic performance while the layer stacking sequence seems to be quite important.[1,7] Different types of non-covalent (van der Waals) and covalent interfaces were studied in the past using atomic layers such as graphene, hBN, MoS_2 etc. Moreover, our recent studies show that some such atomic layer platforms are also interesting in single atom catalysis where they can address the issues related to the existing single atom platforms. Atomic membranes can also play vital roles in mass transfer process, as our recent studies indicated. The talk will be focussing on some of our recent studies on atomic layer interfaces in catalysis and energy storage applications,[8] after giving a brief account of our past works on the related area.

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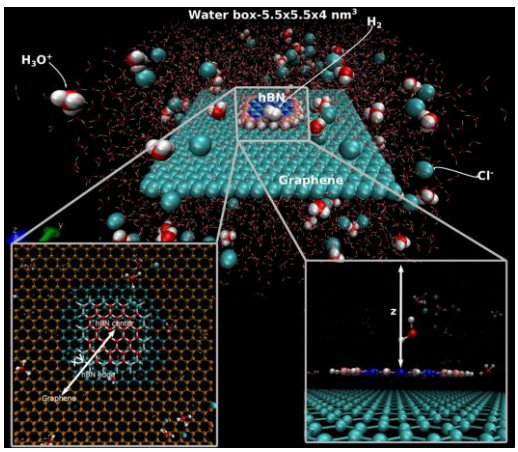

Figure 1: An MD simulation snap shot of Graphene-hBN Interface showing enhanced catalytic (hydrogen evolution reaction) efficacy of the interface.[7]