Title: Hexagonal Boron Nitride (hBN): A Novel 2D Support of Metal Single Atoms for Catalysis

An emergent area in catalysis research is that of single atom catalysis (SAC) due to a decrease in catalyst particle size which results in an increase in chemical activity. Research focused on 2D materials such as hexagonal boron nitride (hBN) has gained traction in recent years for printed devices and coatings, yet as a chemically inert, insulating material, it has not been widely explored as a catalytic substrate. In recent years, studies have shown the introduction of point defects in hBN lattices via mechanical techniques such as cryomilling. The presence of these point defects (e.g. vacancies) in the hBN structure induces chemical activity, thus enabling its use as substrate able to host SACs. In this work, we mechanically introduce vacancies to the hBN lattice. Then, spontaneous reduction at these sites via addition of metal salts, such as platinum chloride, forms metal-BN heterostructures. The activated hBN has been shown to act as an effective support for SAs such as Pt and Cu and was characterized through X-ray Photoelectron Spectroscopy (XPS), high-resolution Transmission Electron Microscopy (HR-TEM), and Extended X-Ray Absorption Fine Structure (EXAFS) to determine the presence of SACs upon the hBN substrate. We explore the spontaneous reduction of the metal salts through a change to the band structure which induces a shift in the Fermi energy, higher than the reduction potential of the metal cations, shown through theoretical calculations. We will demonstrate that these systems have an effective catalytic activity in the hydrogen evolution reaction (HER). The HER data for the Pt-hBN and Cu-hBN samples were collected in an acidic solution (0.5M H_2SO_4) and exhibited very competitive values of overpotentials and a Tafel slopes, outperforming Pt/C catalysts. Thus making SAC-hBN a promising route towards efficient catalytic heterostructures.

[1] Lei, Y.; et. al. *Materials Today,* **2021**, *51*, 108-116