Designing 2D Materials for Hydrogen Production Technologies

Leandro Seixas

MackGraphe, Mackenzie Presbyterian University

Hydrogen is the most abundant element in the universe. About 74% of all matter of the universe is hydrogen (excluding dark matter and dark energy). Our star – the Sun – is 75% hydrogen. On Earth, hydrogen makes 11% of our oceans, and 10% of an average human body. One should note that this element is not generally found on Earth in its molecular form (H$_2$). It is generally bound in larger compounds like organic molecules or water.

Hydrogen is also a source of energy. H$_2$ is the primary source of energy for fuel cells, a device to convert chemical energy into power. These has uses in electric vehicles and static stations for variable renewable energy. Today, the H$_2$ synthesis is usually done through chemical process with fossil fuels (natural gas, oil or coal). These processes have as side effect by-product of carbon dioxide (CO$_2$). Alternative methods as water splitting faces challenges in cost and abundance of the elements that make up the catalysts. For hydrogen production without the greenhouse gases, it is needed to use platinum based catalysts. The use of this rare metal may hinder large-scale deployment of fuel cells and hydrogen production.

In this talk, we present two-dimensional (2D) materials modified by metal adsorption with the purpose of increasing the hydrogen production via electrochemical methods. Tuning the electronic structure and hydrogen free energy, we can optimize the catalytic activity and material stability. We show that metal adsorbed can significantly increase the hydrogen evolution activity of MoS$_2$ monolayers in an unexpected way.