Selective Transport Membrane Electrodes Based on 2D Electronic Materials: new concepts for integrated renewable energy generation

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Electrochemical processes are at the heart of several important energy conversion systems including photoelectrochemical cells for hydrogen generation, energy storage, and electrokinetic water purification systems. While molecular separation membranes consisted of high dielectric constant, low electrical conductivity materials have traditionally used for water purification (polyimide/polysulfone) or proton selectivity (Nafion), there exist several technical hurdles that need to be overcome including bubble formation on electrodes. Therefore, in this project we explored the potential of 2D materials such as MoS_2, graphene and their hybrids in developing bubble-free selective transport membrane electrodes. These materials have electronic properties ranging from metallic to semiconducting, are expected to have enormously high molecular fluxes of gases, and with carefully engineered pores are expected to have excellent selectivity.

In pursuit of this ultimate goal, over the period of this project, thorough investigation into the fundamental physics of the 2D materials was conducted which formed the solid basis to further implement the materials to the target system. We found that there existed an obvious layer number (thickness) dependence of MoS_2 conductivity and photoconductivity when it was in its 2D confinement limit of a single or several layers form. When an interface between different 2D layers was formed (graphene-MoS_2 in this project), we observed a significant charge transfer between the materials and an energy barrier formation at the junction, and demonstrated its artificial modulation. This gained knowledge offers fundamental insights for developing a new type of hybrid 2D composites whose properties can be tuned by modulating the thickness of component materials and the energy barrier to best serve for specific applications. In addition to these electronic and optoelectronic characteristics, the mathematical model we developed describing gas permeation through graphene pores in various limits of gas diffusion, surface adsorption, or pore translocation as the rate-limiting step will further help design selective transport membrane electrodes. We also contributed to large scale production of the 2D materials by experimentally optimizing and mathematically modeling the chemical vapor deposition process for the growth of centimeter-scale high quality MoS_2 crystals. We are now at the stage of transferring the obtained knowledge into practical electrochemical systems using the photo-electrochemical workstation in the water splitting laboratory at the Kuwait Institute of Scientific Research (KISR) which is still ongoing efforts. However, the results should not be limited to the electrochemical systems we are aiming for, and any researchers who may be interested in taking advantages of unique properties of 2D materials for any of their systems will benefit from the outcomes of the project.