**Molecular Dynamics Simulations Reveal that Water Diffusion between Graphene Oxide Layers is Slow**

**Objective**

The main objective of this research paper was to check Graphene oxide simulation at different hydration levels. One of the objectives is to synthesize the GO layer in lab and perform its molecular dynamics study.

**Methodology**

**Lab work:**

They synthesized membranes from a range of different GO sources with the goal of obtaining various flake sizes, from 100 nm to 100μm in nominal diameter. They used a simple solution filtration and casting on a polytetrafluoroethylene plate (12” × 12”) to isolate free-standing GO membranes. In addition to the variable flake sizes, they prepared membranes with thicknesses ranging from 5μm to 50μm and characterized them using multiple measurement techniques including X-ray diffraction pattern to detect the change in layer spacing that accompanies changes in mass and thickness of GO with changes in the hydration level.

**Simulations:**

They performed classical molecular dynamics simulations of GO membranes with H2O using the DLPOLY4 computer code. They used the DREIDING force field to describe the GO  
layer, the F3C potential for H2O, and the non-bonded interaction parameters for the C-H2O interactions. They used harmonic bond stretching and angle bending terms with bond lengths and bond angles constrained to correspond to the relaxed GO structure. The simulation cell contained three layers of GO and was periodically repeated in all dimensions.

**Findings**

Results showed that water diffusion in GO is an order of magnitude slower than in bulk water due to strong hydrogen bonded interactions between H2O molecules and the OH group. Even at the highest hydration level of 23.3 wt.% H2O, only about 21% of the H2O molecules were free or bulk-like. They observed large water clusters comprising 10 to 30% of the water molecules present in the system. Such clusters can span across oxidized regions, graphitic regions, and defects or holes that have been seen in experiments thereby contributing to rapid water transport.