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"Aqueous Proton Transfer Across Single-layer Graphene"

Proton transfer across single layer graphene is associated with large computed energy barriers and is therefore thought to be unfavorable at room temperature. Experiments, however, have not yet been performed to test this prediction. Here, we subject single layer graphene on fused silica to cycles of high and low pH and show that protons transfer reversibly from the aqueous phase through the graphene to the other side where they undergo acid-base chemistry with the silica hydroxyl groups. After ruling out diffusion through macroscopic pinholes, the protons are found to transfer through rare, naturally occurring atomic defect sites. Computer simulations reveal low energy processes for water-mediated proton transfer across hydroxyl-terminated atomic defect sites that participate in a Grotthuss-type relay, while defects terminated by pyrylium-like ether bridges shut down proton exchange. Unfavorable energy barriers to helium and hydrogen transfer indicate that single layer graphene is selectively permeable to aqueous protons.

MATERIALS SEMINAR

Monday, March 16th at 3:30 p.m. in Seminar Hall (1315 Chemistry)