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Speaker

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Talk Title

Tuning Proton Transfer and Hydrogen Isotope Selectivity in Graphene

Abstract

Atomically thin graphene is a promising platform for proton transport and hydrogen isotope separation due to its impermeability to most atoms combined with its ability to permit proton permeation under appropriate conditions [1]. Experiments by Lozada-Hidalgo and co-workers demonstrated that monolayer graphene can effectively separate hydrogen isotopes, achieving an H^+/D^+ separation factor of approximately 10 at room temperature [2]. However, graphene membranes under realistic conditions are neither structurally nor electronically uniform. Ripples, wrinkles, strain, local chemical modifications, and external electric fields can alter the local environment experienced by a proton and thereby strongly affect its transfer across the membrane [3,4].

In this work, we investigate how the proton-transfer barrier through graphene can be controlled by three complementary strategies: mechanical deformation, external electric fields, and atomic substitution. We first examine biaxial tensile strain and local out-of-plane curvature, showing how changes in the carbon framework modify the transfer barriers and isotope selectivity for H^+ , D^+ , and T^+ . Tensile strain increases the available space within the carbon lattice and progressively lowers the proton-transfer barrier, while local curvature provides an additional means of tuning proton permeation through nanoscale structural deformation. We further explore how an applied electric field modifies the energetics of proton transfer and how substitution of selected carbon atoms with B and/or N atoms alters the local electronic structure and interaction with the transferring proton. Together, these results demonstrate that proton transport

through graphene can be systematically tuned through both structural and electronic modifications, providing microscopic insight into strategies for controlling proton conductivity and hydrogen isotope selectivity in atomically thin membranes.

References

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Short biography

Agnieszka Kuc graduated from Wroclaw University in 2003 with an M.Sc. in physical chemistry (supervisors: Prof. Koll and Dr. Filarowski). She completed her Ph.D. in chemistry under the supervision of Prof. Gotthard Seifert at TU Dresden in 2008. She habilitated in Physics in 2018 under mentoring of Prof. Thomas Heine at Jacobs University Bremen. She is currently working as a group leader at Center for Advanced Systems Understanding (CASUS), Helmholtz-Zentrum Dresden-Rossendorf. Her research interests include, among others, electronic structure simulations and vibrational properties of 2D inorganic and hybrid materials, such as transition-metal dichalcogenides, conjugated polymers, metal- and covalent organic frameworks, and perovskites, their 2D heterostructures, as well as proton transport and hydrogen isotope separation using graphene membranes.