

Effects of Mechanical Strain and Local Curvature on Hydrogen Isotope Selectivity in Graphene Membranes

Maria Judith Caisachana Lozada¹, Ismail Eren³, Agnieszka Beata Kuc^{2,3}

¹Helmholtz-Zentrum Dresden-Rossendorf, HZDR, Institute of Resource Ecology, Permoser Strasse 15, 04318 Leipzig, Germany

²Helmholtz-Zentrum Dresden-Rossendorf, HZDR, Bautzner Landstrasse 400, 01328 Dresden, Germany

³Center for Advanced Systems Understanding, CASUS, Conrad-Schiedt-Strasse 20, 02826 Görlitz, Germany

Email: m.caisachana-lozada@hzdr.de

Atomically thin graphene is a promising platform for hydrogen isotope separation due to its impermeability to most atoms and selective proton permeation [1]. Experiments by the Lozada-Hidalgo group have reported permeation velocity ratios of approximately $H^+/D^+ \approx 10$, $H^+/T^+ \approx 30$, and $D^+/T^+ \approx 2$, which demonstrate isotope-dependent selectivity [2]. Under environmental conditions, graphene membranes are not perfectly flat [3]. Thermal fluctuations and hydration forces induce intrinsic in-plane and out-of-plane corrugations. Experimental studies have shown that high-proton-conductivity regions are observed near ripples, wrinkles, and strained regions, indicating that local lattice deformation is a key factor in hydrogen isotope transfer [4]. In this work, we investigate how controlled biaxial tensile strain (1–5%) and local curvature influence isotope selectivity (H^+ , D^+ , T^+) in graphene membranes. Moderate tensile strain enlarges interatomic spacing and reduces the activation barrier for proton transfer, while local curvature modulates the barrier depending on its out-of-plane deformation. The results provide insight into how biaxial strain and ripples can modulate proton conductivity and isotope separation performance in graphene membranes.

References

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