Angstrom-Size Pore Creation and Ionic Transport through in Single-Layer MoS$_2$

Jothi Priyanka Thiruraman$^{1,2}$
Marija Drndic$^1$

$^1$Department of Physics and Astronomy, $^2$Department of Electrical and Systems Engineering, University of Pennsylvania, Philadelphia, PA 19104, United States

jothi@seas.upenn.edu, drndic@physics.upenn.edu

Atomic-defect engineering in thin membranes provides opportunities for ionic and molecular filtration and analysis. While molecular-dynamics (MD) calculations have been used to model conductance through atomic vacancies, corresponding experiments are lacking. We create sub-nanometer vacancies in suspended single-layer molybdenum disulfide (MoS$_2$) via Ga$^+$ ion irradiation, producing membranes containing $\sim$300 to 1200 pores with average and maximum diameters of $\sim$0.5 and $\sim$1 nm, respectively. Vacancies exhibit missing Mo and S atoms, as shown by aberration-corrected scanning transmission electron microscopy (AC-STEM). The longitudinal acoustic band and defect-related photoluminescence were observed in Raman and photoluminescence spectroscopy, respectively. As the irradiation dose is increased, the median vacancy area remains roughly constant, while the number of vacancies (pores) increases. Ionic current versus voltage is nonlinear and conductance is comparable to that of $\sim$1 nm diameter single MoS$_2$ pores, proving that the smaller pores in the distribution display negligible conductance. Consistently, MD simulations show that pores with diameters <0.6 nm are almost impermeable to ionic flow. Atomic pore structure and geometry, studied by AC-STEM, are critical in the sub-nanometer regime in which the pores are not circular and the diameter is not well-defined. This study lays the foundation for future experiments to probe transport in large distributions of angstrom-size pores.