

## SALT-EXCLUDING ARTIFICIAL WATER CHANNELS EXHIBITING ENHANCED DIPOLAR WATER AND PROTON TRANSLOCATION

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Aquaporins (AQPs) are biological water channels known for fast water transport ( $\sim 10^8$ - $10^9$  molecules/s/channel) with ion exclusion. Few synthetic channels have been designed to mimic this high water permeability, and none reject ions at a significant level. Selective water translocation has previously been shown to depend on water-wires spanning the AQP pore that reverse their orientation, combined with correlated channel motions. No quantitative correlation between the dipolar orientation of the water-wires and their effects on water and proton translocation has been reported. Here, we use complementary X-ray structural data, bilayer transport experiments and molecular dynamics (MD) simulations to gain key insights and quantify transport. We report artificial imidazole-quartet water channels with 2.6-Å pores, similar to AQP channels, that encapsulate oriented dipolar water-wires in a confined chiral conduit. These channels are able to transport  $\sim 10^6$  water molecules per second, which is within two orders of magnitude of AQPs' rates, and reject all ions except protons. The proton conductance is high ( $\sim 5$  H<sup>+</sup>/s/channel) and approximately half that of the M2 proton channel at neutral pH. Chirality is a key feature influencing channel efficiency.

