

NANO HOUR

Wednesday, January 24, 2007

3:00 PM

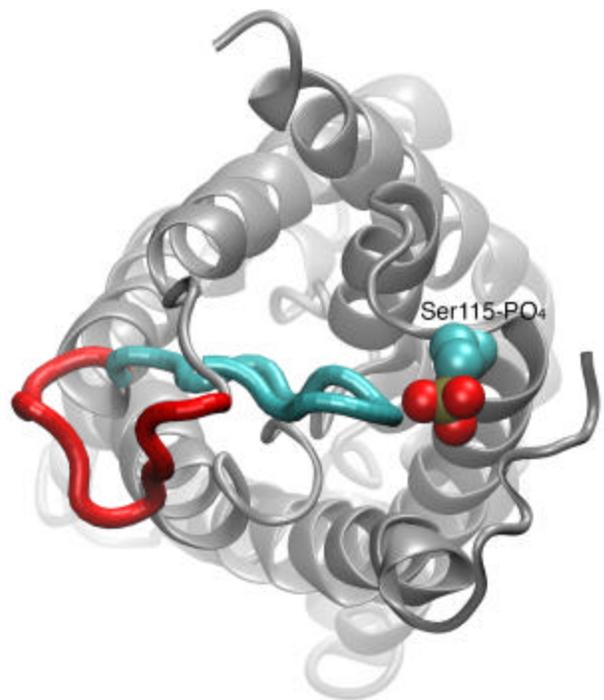
Beckman Institute - Room 3269

Exploring Gas Permeability and Gating Mechanism of Aquaporins

Yi Wang

Graduate student in Biophysics and Computational Biology working with the Theoretical and Computational Biophysics Group in the Beckman Institute.

Aquaporins (AQPs) are a family of membrane proteins specializing in rapid water transport across biological membranes. Whether these water channels can also conduct gas molecules has remained a long-standing question. Using molecular dynamics simulations, we studied the permeability of human AQP1 to two types of gas molecules, O₂ and CO₂. The central (tetrameric) pore of AQP1 was identified as a pathway for both gas molecules to cross the membrane. Molecular dynamics simulations were also used to explore the gating mechanism of a plant aquaporin. In a 15 ns simulation, the spinach aquaporin SoPIP2;1 was found to switch from a closed state to an open state upon phosphorylation. Two complementary mechanisms governing the gating process were revealed by the simulation.



Coffee and cookies will be served.

<http://nanohour.beckman.uiuc.edu>