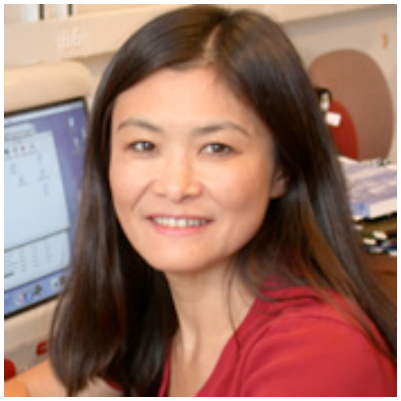
Physical Chemistry Seminar

Tuesday, April 28, 2015 | **11:00 am** | **Room 1315 Chemistry Building**

What Makes Water Unique? A Molecular Perspective



Professor Toshiko Ichiye

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Host: Professor Qiang Cui

Although water is the most ubiquitous liquid on this planet and is necessary for life, the molecular basis for its unique properties is still not completely understood. Atomistic modeling of water in computer simulations is often used to examine how water molecules behave as a liquid and a solvent. However, determining the *minimal* molecular features in an empirical potential energy function for water that are necessary to reproduce its unique properties provides insight into what the *essential* molecular features are. Given the myriad of potential energy functions, here we determine which features are necessary to reproduce multiple structural, dynamic, and electrostatic properties of liquid water and are also consistent with quantum mechanical calculations. In addition, we examine how these molecular features determine the nature of the long-range tetrahedral network of hydrogen-bonded water molecules. Finally, we examine how solutes and surfaces disrupt the network.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8305F