The 80th MANA Special Seminar

Charges in solution: Physics and Chemistry of a perturbed hydrogen bond network probed by first-principles molecular dynamics.

Chair: Dr. Takahisa Ohno (Computational Materials Science C)

Prof. Mauro Boero

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An overview on recent first-principles molecular dynamics simulations, focusing on charged objects in water solution, shows how simulations can complement experimental results, providing the information not directly accessible to experimental probes. At the same time, this kind of approach is suitable to make predictions and to be used as a tool to perform virtual experiments. In this talk, I shall present a general overview, ranging from simple unit charges (electron and proton) in water to more complex ions (Na+, Cl-, etc.), showing how the atomic-level picture given by simulations can be used to extract macroscopic observable quantities experimentally detectable. This specific research theme, which was done in collaboration with NIMS (ICYS and MANA), is shown to be interdisciplinary, with implications ranging from solution chemistry to biology.

Venue: **Seminar Room #431, MANA Bldg.**

Date: **May 27th Wednesday** ***Time:*** **15:30-16:15**

NAMIKI Site

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