ABSTRACT
Aqueous electrolyte solutions play an important role in chemical engineering separations, in geochemical environments and for biophysics. The mean ionic activity coefficients quantify the deviation of salt chemical potential from ideal solution behavior; experimental measurements are available over broad ranges of concentration and temperature, but there have been practically no prior simulation results of these quantities, because of sampling difficulties for explicit-solvent electrolyte solutions. We have developed a reliable approach for determination of activity coefficients of aqueous electrolytes. Common fixed-point-charge models for water and ions are unable to reproduce simultaneously activity coefficients and solubilities, especially at elevated temperatures. Polarizable models perform better, but still predict an incorrect temperature dependence of these properties. In addition, we have found significant finite-size effects on these properties that need to be corrected for to obtain accurate activity coefficients. We have used forward-flux-sampling and metadynamics methods to obtain insights on the nucleation rates and pathways for NaCl crystallization from supersaturated aqueous solutions and to compare different salt and water models with respect to their ability to describe experimental measurements.

BIOGRAPHY
Thanos Panagiotopoulos received an undergraduate degree from the National Technical University of Athens and a PhD from MIT, both in Chemical Engineering. After a postdoctoral in Physical Chemistry at the University of Oxford, he has held faculty positions at Cornell and the University of Maryland; he is currently the Susan Dod Brown Professor and Department Chair of Chemical and Biological Engineering at Princeton University. He is a member of the U.S. National Academy of Engineering and the American Academy of Arts and Sciences. He is the author of more than 280 technical articles and of the undergraduate textbook “Essential Thermodynamics.”