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Rate Theory on Ion Pairings at the Liquid/Vapor Interface of Water LIEM DANG, Pacific Northwest Natl Lab — There is overwhelming evidence that ions are present near the vapor–liquid interface of aqueous salt solutions. Despite their importance in many physical phenomena, ways in which ion–ion interactions and related properties, such as the kinetics and thermodynamics, are affected by interfaces have not been quantified. We use molecular simulations to exam the thermodynamics and kinetics of small alkali halide ions in the bulk and near the water vapor–liquid interface. We will calculate dissociation rates using transition state theory, and weight them with transmission coefficients determined by the reactive flux method and Grote-Hynes theory. Our results will show that, in addition to affecting the free energy of ions into solution, the interfacial environments (i.e., redistribution of the hydrogen bonds network) and the anion type should significantly influence the kinetics of ion pairings. These results will increase our understanding of thermodynamic and kinetic properties of ion pairing in different environments.

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