Public Abstract
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We use computational methods to examine two systems of practical interest in our study. In the first, we use a novel method to characterize heat exchange between a gas and a liquid surface. The results of this study provide a framework for elucidating the combustion of liquids as well as for understanding the general interactions of gases with liquids. In particular, we are able to determine both the average heat exchange between a molecular gas and a prototypical liquid surface and typical dynamical events that yield the net energy transfer. Our second study examines the motion of gas particles through liquids of current technological interest. This study has applications to gas storage as well as to reactivity of gases in these unusual liquid systems. Our model is able to approximate the properties of the liquid, including the unique spatial layering that results from the liquid's ionic character. Our determination of the average motion of gas species within this liquid, obtained using two independent models, agrees reasonably well with existing literature results, thereby further encouraging explorations of these systems.