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Structure and Adsorption on Hydrated Alumina Surfaces VINCENZO LORDI, PATRICK HUANG, ERIC SCHWEGLER, Lawrence Livermore National Lab — Understanding the mechanisms of adsorption of chemical agents on environmental materials under different atmospheric conditions is important for applications in environmental remediation, industrial catalysis, and protection against chemical warfare. In this work, we study molecular adsorption of the chemical agent simulant dimethyl-methylphoshonate (DMMP) on various alumina surfaces, using density functional theory-based molecular dynamics simulations. Both alpha and gamma alumina surfaces of different orientations (and thus surface terminations/reconstructions) are studied, under both wet and dry conditions. Adsorption from the gas phase onto dry and hydroxylated surfaces is compared to adsorption from an aqueous layer in the limit of a fully bulk-like liquid water layer. Interfacial structure and dynamics are directly compared to previous synchrotron X-ray scattering and sum-frequency vibrational spectroscopy experiments, from which specific contributions of different surface functional groups are identified and resolved. Differences in site reactivity on the various surfaces are also compared. Prepared by LLNL under Contract DE-AC52-07NA27344.

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