

Abstract Submitted  
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**Molecular Dynamics Investigation of the Products of Alkoxysilane Condensation: Bulk Gels and Surface Coatings** ROLAND FALLER, JOSHUA DEETZ, UC Davis — We characterize silica gels and organo-silicon surface coatings using reactive molecular dynamics simulations. To model the chemical reactions, we use a reactive force field (ReaxFF) which we have optimized in a novel parallelized semi-automatic way to model hydrolysis and condensation reactions. The morphologies of silica gels obtained from tetra- and tri-alkoxysilanes are determined by allowing the system to condense while simultaneously removing water and replacing it with precursor solution. It is found that the gels obtained from trialkoxysilanes are more loosely bonded, and that the chemistry of the headgroup is important to the gel morphology. We furthermore simulated the chemisorption of alkoxysilanes with organic headgroups to hydroxylated silica surfaces. We observe a competition between alkoxysilanes condensing with themselves or with the silica surface.

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