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**The Effect of Solvent and Precursor Functionalization on the Fractal Dimension and Physical Properties of Sol-Gel derived Silica**  
SUDIN BHATTACHARYA, JOHN KIEFFER, Materials Science and Engineering, University of Michigan — We have used molecular dynamics simulations based on a recently developed three-body charge-transfer potential to simulate sol-gel condensation reactions that produce nano-porous silica gel structures. The effect of solvent molecules on the fractal dimension of the gels prior to, and after, supercritical drying is investigated. With pure silicic acid monomer precursors, the sol-gel aggregation process produces fractal 3-D network structures. However, with silicic acid dimers and dimers functionalized with cyclohexyl groups, closed cage-like structures are observed prior to further polymerization into a network. We examine how this structural variation affects the fractal dimension and structure-property relationships of the system.

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