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Abstract Formulary

Presentation type: **Oral** ✔ **Poster** ☐

Title: Insights into colloidal aerogel structures from diffusion limited mixed aggregation

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ABSTRACT (Space limited to 2200 characters)

Knowledge of the microstructure of aerogels can help with optimization of the relevant physical properties for a specific target application such as superinsulation, Knudsen pumps, etc. Experimental results need to be supplemented with computational methods in order to get a complete picture of the 3D microstructure and the pore landscape. The current state-of-the-art methods for colloidal aerogels are based on Diffusion-Limited Cluster Aggregation (DLCA) algorithms, showing qualitative fit with Small-Angle Scattering (SAS) experiments. In the present work, we propose a Diffusion-limited Mixed Aggregation algorithm that recovers the Diffusion Limited Aggregation (DLA) and DLCA classes of structures in different limits in a 3D off-lattice truly periodic system. This approach thereby accounts for the local cluster growth in the gelation process and is capable of generating a vast array of structures by tuning the parameters. We study the percolation limits of and the theoretical small-angle scattering curves produced by these structures in the entire parameter space. Furthermore, we calculate pore size distribution, specific surface area and density and compare to experimental values for Tetraethyl orthosilicate based aerogels (with porosity ranging between 87%-96%) to determine the relevant parameter space and the corresponding microstructure of the samples. The aim is a unifying model for both small angle scattering and physisorption data. We will be putting our models in context with previously reported models in literature, discuss the current theoretical limitations and sketch ways towards better structural models and an improved understanding of the aerogel pore landscape.