Molecular mechanisms of mesoporous silica formation from colloid solution

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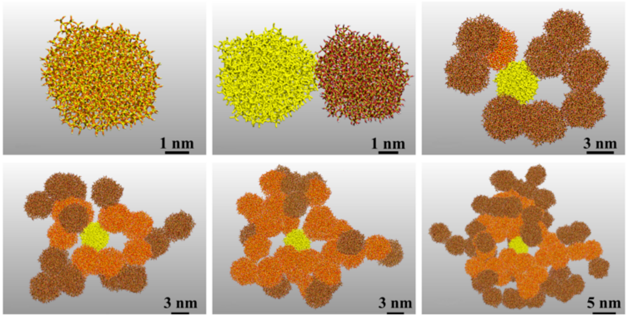
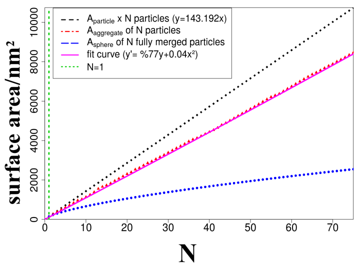
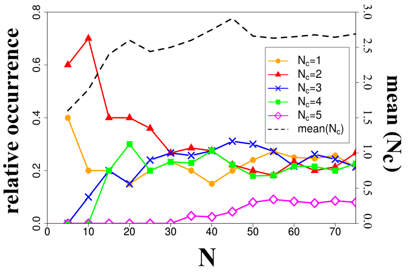
Silica particles and nanocomposites are being used in many applications ranging from catalysts to coatings, reinforced plastics and recent studies suggested silica nanomaterials to be used as biocatalyst,drug/gene delivery vehicles, and also for biomimetic processes like bone tissue engineering. For bionanotechnological applications, colloidal amorphous silica is taken as a base material to form mesoporous silica. Considering huge demand of silica nanomaterials, understanding and controlling interfacial interactions, association and aggregation is vital to the goal-oriented use of colloidal silica particles.



In this work, we investigated the agglomeration of silica nanoparticles in aqueous solution from molecular simulations through colloidal silica association of $SiO_2/Si(OH)_4$ core/shell particles, local silanole → silica ripening reactions within a limited contact zone and finally the formation of mesoporous precipitates. This calls for profound characterization of molecular interactions and the assessment of extended relaxation processes at the same time. To cope with the inherent time-length scale challenge to molecular simulation, we employ the Kawska-Zahn approach [1,2]. Implementing sufficiently fast supply from colloidal solution, our simulations show the development of silica networks comprised of covalently bound, yet not fully merged nanoparticles in which coordination numbers range from 2 to 5 and with 77% theoretical limit of porosity – which is far from the closest packing.





[1] A. Kawska, J. Brickmann, R. Kniep,O. Hochrein,D. Zahn, *J Chem Phys*,**2006,**124,24513

[2] A. Kawska, J. Brickmann, R. Kniep,O. Hochrein,D. Zahn,*ChemPhysChem*, **2010,** 11,847-852.