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# Computer-aided Design of Bio-inspired Nanoporous Silica Materials

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July 15, 2015

# 1 Summary

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## 2 Acknowledgements

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### 3 Introduction

Molecular Dynamics (MD) and Monte Carlo (MC) are powerful tools to simulate molecular interactions of surfactants in solvent systems, allowing a deeper understanding of their self-assembly process (?). This process results in several types of surfactant mesoscale conformations that are specially useful to design bio-inspired silica materials (?). With the addition of silica, these structures behave as scaffolds to mesoporous or nanoporous structures that are maintained even after surfactant removal, silica oligomer polymerization and calcination (?). A vast range of silica materials are examples of this phenomena, such as MCM-41 as reported by ? (?), SBA-15 (?), MSU-V (? ) and many others, in which the self-assembled structure depends on the type of surfactant, concentration of the substances involved and synthesis conditions such as temperature and pH. It should be noted that most of the experimental methods used to obtain data are based on observation and interpretation of final silica structure by using X-ray diffraction (XRD) and transmission electron microscopy (TEM). It follows that initial self-assembled conformations are predicted as a reflex of the final results and little is known about the mechanistic of this process. However, with MD simulations it is possible to observe and analyse these initial steps of self-assembly and predict, with more accuracy, properties and frameworks provided by surfactants (?).

On the other hand, a major concern is that even though MD uses sophisticated software prepared to simulate systems with thousands of atoms, using all capacities of hardware available, such as high-speed multi-core processors in conjunction with GPUs designed specifically to process data from arrays (?), they can hardly achieve long time horizons and are commonly limited to a few microseconds depending on the size of the system. For this reason, several techniques have been developed to optimize the performance of the simulations such as coarse-grain methods (?). The basic idea of this technique is to fit parameters of atom groups with similar properties in a bigger "bead", which includes atomic masses and electrostatic charges lumped in approximated values. For example, given a simulation of an arbitrary surfactant with a long hydrophobic tail, it is possible to merge three or four carbon atoms (and its hydrogen atoms) in groups since they have similar hydrophobic properties, by this means reducing the number of particles in the system and speeding up the simulation.

In order to provide molecular topologies to simulations software packages several force-fields, for example MARTINI (?), uses Lennard-Jones potentials fitted to a range of pre-defined bead types to describe coarse-grain models. Furthermore, not only intramolecular beads are possible, but also intermolecular beads can be specified, such as multiple solvent molecules merged in a single bead or ions surround by water molecules. Previous works conducted by (? ) with this method recreated a model of surfactant in the presence of silica with explicit water that was successful in describing rod-like self-assembly structures detected on MCM-41 materials, demonstrating the capacities of up-scaling this type of systems. Nevertheless, solvent presence demands most of the computational resources, hence implicit solvent scheme has been the focus of many studies (?).

Different concepts have been applied to develop a suitable model for implicit solvents; For example, ? (?) developed the Dry MARTINI force-field by modifying parameters of its predecessor, in such manner that solvent interactions became incorporated in these values and then solvent beads are no longer necessary. Another method, described by ? (?) is able to recreate an implicit solvent system from interaction potentials generated from a bottom-up approach, that means by using an all-atoms simulation to generate parameters for the coarse-grain model. It is supposed that thermodynamic changes on the system, originated from solvent interaction with amphiphilic molecules, are incorporated in these approximated potentials. Therefore, changes in parameters as concentration may not affect coarse-grained model performance in recreating self-assembly structures (?).

The work presented in the following experiments is an attempt to create a flexible method to upscale silica-surfactant interactions (? ) from the atomistic model to a mesoscale model with the advent of this later coarse-grain technique. The methodology applied to reach the desired model is based on the MagiC software package (? ) that in conjunction with a MD simulation software, in this case GROMACS (?), will provide a suitable approximation to self-assembly of amphiphilic molecules. Further explanations of the process are described in the Experimental Methods section. For the scope of this project, a bolaamphiphilic molecule called 1,12-diaminododecane (DMDD) has been chosen as surfactant because, as seen in previous research by ? (?), it self-assembles in multilamellar vesicles that in the presence of a silica precursor are capable of generating a mesoporous structure with remarkable properties. In order to validate this structure formation and framework formation for silica oligomers, a coarse-grain approximation is a suitable option since amphiphilic molecules interaction with solvents can be described efficiently with tabulated Lennard-Jones potential interactions. As a final objective at the end of this project, an implicit water coarse-grain model for DMDD will be generated and properly validated based on MD simulations and thermodynamic properties, in order to provide a satisfactory

approximation to interactions with silica oligomers in a mesoscale model.

## 4 Theoretical Basis

## 5 Methods Description

## 6 Results and Discussion

## 7 Conclusion

## 8 Nomenclature

$k_B$	Boltzmann's Constant
$C_n$	Molar concentration of species n ( $mM$ )

## 9 References

Need, A., & Someone, T. C. (2025). Mock article: You need to read more. *Journal of Void Theory*, 1(1), 151-1510.

## 10 Appendix