Computational Materials Science

Soft-Matter Multiscale Simulations

Self-assembly of Triton X-100 in water solutions

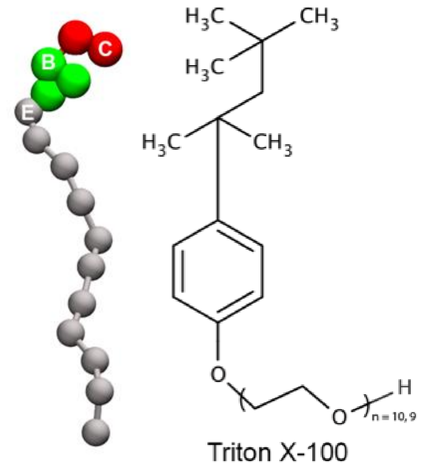
A multiscale scheme is proposed and validated for Triton X-100 (TX-100), which is a detergent widely employed in biology. The hybrid particle field formulation of the model allows simulations of large-scale systems. The coarse-grained (CG) model, accurately validated in a wide range of concentrations, shows a critical micelle concentration, shape transition in isotropic micellar phase, and appearance of hexagonal ordered phase in the experimental ranges reported in the literature.

The fine resolution of the proposed CG model allows one to obtain, by a suitable reverse mapping procedure, atomistic models of micellar assemblies and of the hexagonal phase. The proposed model opens the way to investigations of several mechanisms involving TX-100 assembly in protein and membrane biophysics.

[J. Chem. Theory Comput. 2015, 11, 4959−4971]

Hybrid model of Triton X-100

The molecular models considered here were developed in a hybrid MD-SCF scheme combining particles and field representations for nonbonded interactions. In the frame of self-consistent field (SCF) theory, the interaction of a particle with other nonbonded particles is considered only through a mean field.



Triton X-100

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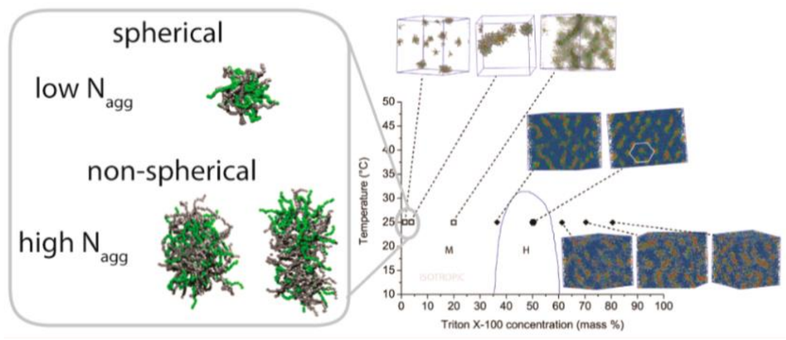
Results

A coarse-grained (CG) model is proposed and validated for TX-100. The hybrid particle field formulation of the models allows simulations of large-scale systems (having beads number ranging from 100.000 to 600.000 for simulation times from 5 μs to 15 μs). The CG model has been accurately validated in a wide range of concentrations in aqueous solution.

The proposed model, because of its computational efficiency for parallel applications, opens the way to investigations of several mechanisms involving TX-100 assembly in protein and membrane biophysics.

All MD simulations have been performed thanks to CRESCO 4 HPC infrastructure.



Biomembrane Solubilization Mechanism by Triton X-100: A Computational Study of The Three Stage Model

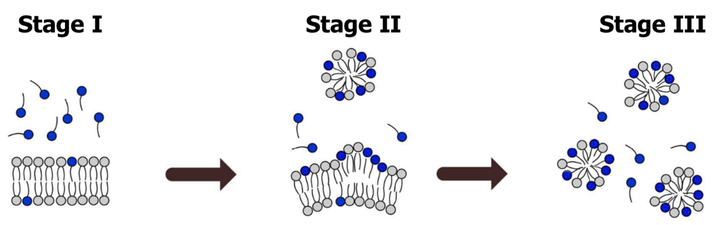
The solubilization mechanism of lipid membrane in presence of Triton X-100 (TX-100) is investigated at molecular resolution by Molecular Dynamics (MD) simulations. Thanks to the large time and length scales accessible by the hybrid particle-field formulation of the models here employed, the complex process of membrane solubilization has been studied, with the goal of verifying the literature Three Stage Model. DPPC lipid bilayers and vesicles have been studied at different concentration of TX-100 detergent employing Coarse Grained (CG) models. Systems up to ~ 600.000 beads, corresponding to more than 2 millions of heavy atoms, have been simulated. Moreover, in order to clarify several experimental evidences, both slow and fast detergent partitions scenarios have been investigated.

MD-SCF Approach, CG Models

The main feature of the hybrid MD-SCF approach is that the calculation of intermolecular non-bonded forces and potentials, representing the most computationally demanding part of MD simulations, can be substituted by a calculation of external potentials dependent on the local density, sa reported in the following equation(G. Milano and T. Kawakatsu, *The Journal of Chemical Physics*, **2009**, 130, 214106):

$$W[\{\phi_K(\mathbf{r})\}]\int d\mathbf{r}\left(\frac{K_BT}{2}\sum_{KK'}\chi_{KK'}\phi_K(\mathbf{r})\phi_{K'}(\mathbf{r})+\frac{1}{2\kappa}\left(\sum_K\phi_K(\mathbf{r})-\phi_0\right)^2\right)$$

The aim of the work is to study very complex biiological phenomena such as three stage model (reported in the figure below).



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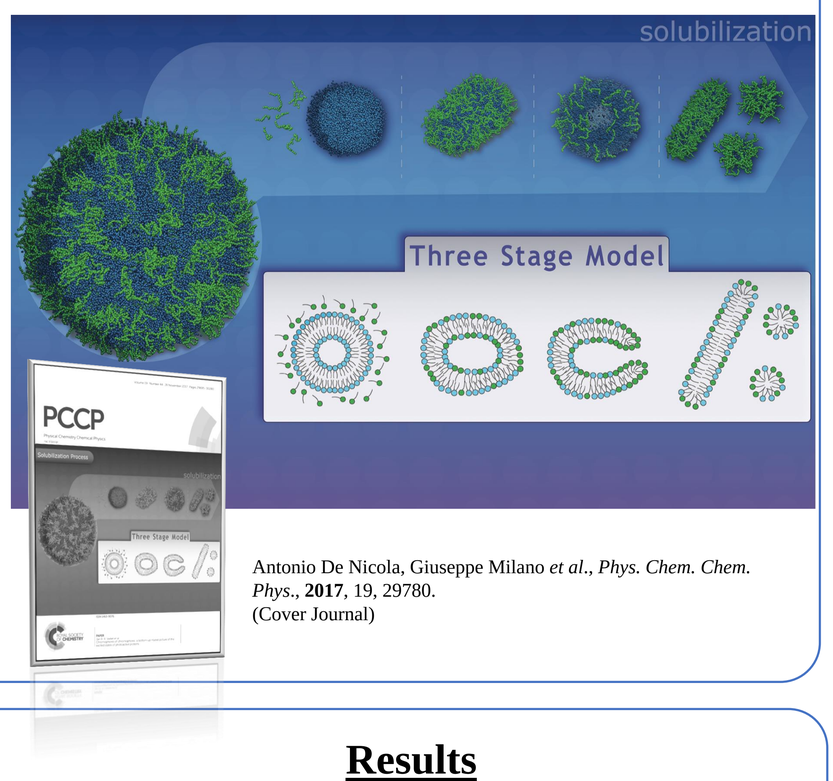
Results

The solubilization of a lipid membrane by Triton X-100 is investigated at molecular resolution using molecular dynamics simulations. Thanks to large time and length scales accessible by the hybrid particle–field approach, it is possible to monitor the whole process, and to confirm the three stage model for the solubilization mechanism.



Antonio De Nicola, Giuseppe Milano *et al.*, *Phys. Chem. Chem. Phys.*, **2017**, 19, 29780.
(Cover Journal)

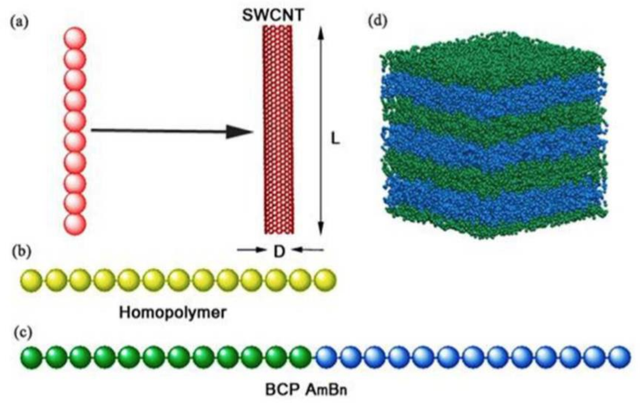
Self Assembly of carbon nanotubes in polymer melts: structural and electrict properties from MD simulations

Self-assembly processes of carbon nanotubes (CNTs) dispersed in different polymer phases have been investigated using a hybrid particle-field molecular dynamics technique (MD-SCF). This efficient computational method allowed simulations of large-scale systems (up to ~1 500 000 particles) of flexible rod-like particles in different matrices made of bead spring chains on the millisecond time scale. The equilibrium morphologies obtained for longer CNTs are in good agreement with those proposed by several experimental studies that hypothesized a two level “multiscale” organization of CNT assemblies. In addition, the electrical properties of the assembled structures have been calculated using a resistor network approach. The calculated behaviour of the conductivities for longer CNTs is consistent with the power laws obtained by numerous experiments.

Model

All simulations (MD-SCF) reported have been performed using the parallelized version of the OCCAM MD code(1), moreovoer, thanks to the HPC CRESCO 4 optimization, has been possible to perform simulations up to $1.5x10^6$ atoms.

Respresntation of block-copolymer and carbon nanotubes, having different aspect ration, are reported in the figure below.



CG model of (a) CNT; (b) homopolymer chain; (c) symmetric block copolymer chain AmBn, with A bead (green) that is compatible with the CNT. (d) block copolimer template system.

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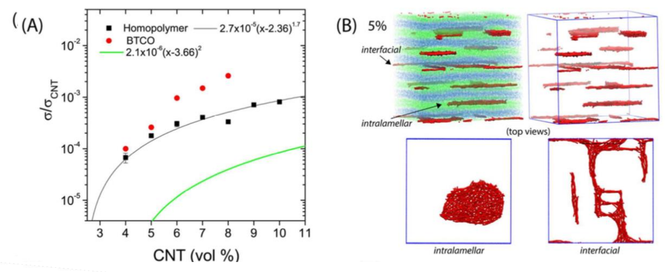
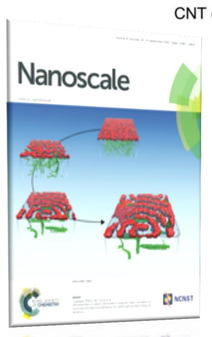
Results

The self-assembly processes of CNTs in different polymer matrices have been simulated for large-scale systems. The equilibrium morphologies obtained for longer CNTs are in good agreement with those ones proposed on the basis of experimental data. Electrical properties of the assembled structures have been calculated using a resistor network approach, and the calculated conductivity behaviours for longer CNTs are consistent with experiments.





OCCAM Molecular Dynamics

(1) Y. Zhao, A. DeNicola, T. Kawakatsu and G. Milano, *Journal of Computational Chemistry*, **2012**, 33, 868-880
occam website: www.smms.unisa.it/occam

Self-Assembly of Carbon Nanotubes in Polymer Melts: Simulation of Structural and Electrical Behavior by Hybrid Particle-Field Molecular Dynamics , *Nanoscale*, **2016**, 8, 15538-15552
(Cover Journal)

Computational MAterials Science & Technology (CMAST) Virtual Lab http://www.afs.enea.it/project/cmast/