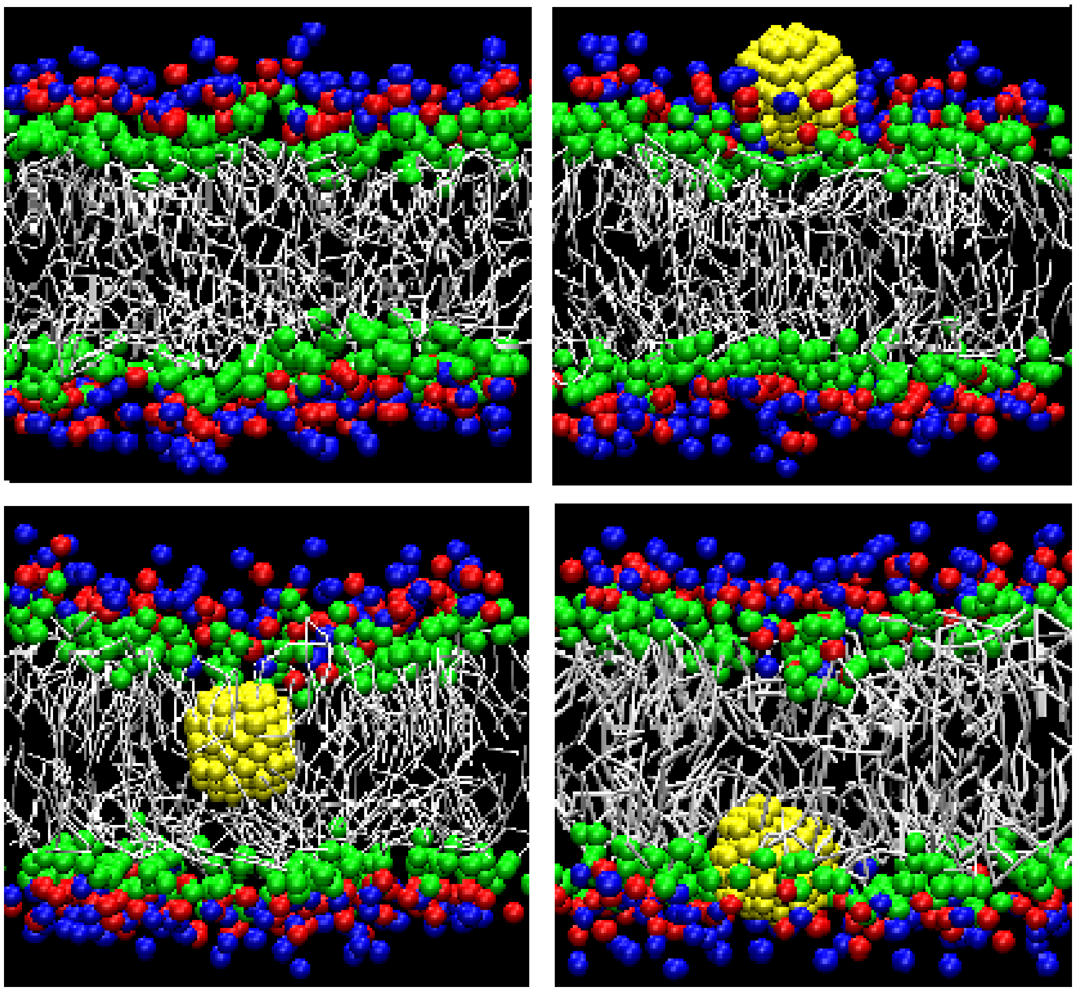
Gold nanocrystals at DPPC bilayer



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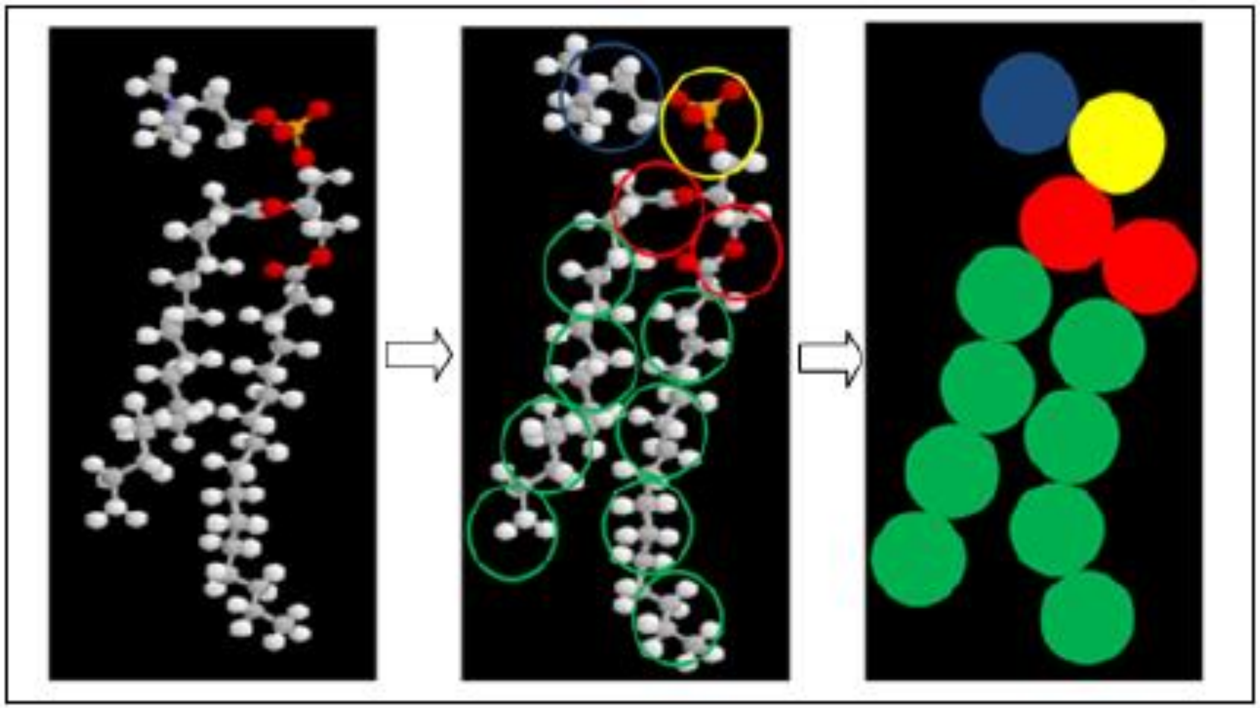
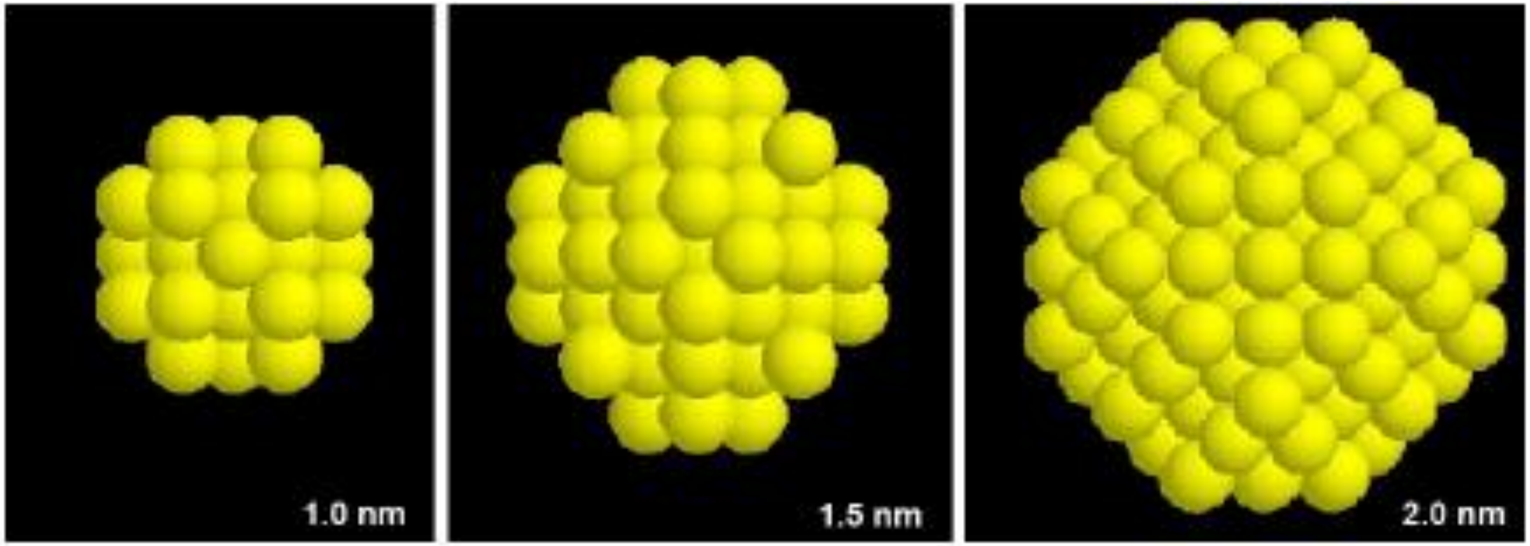
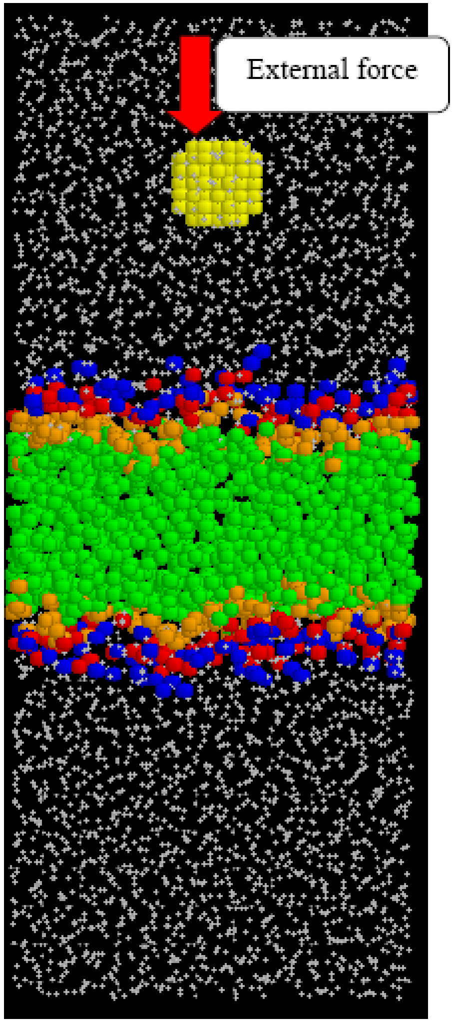


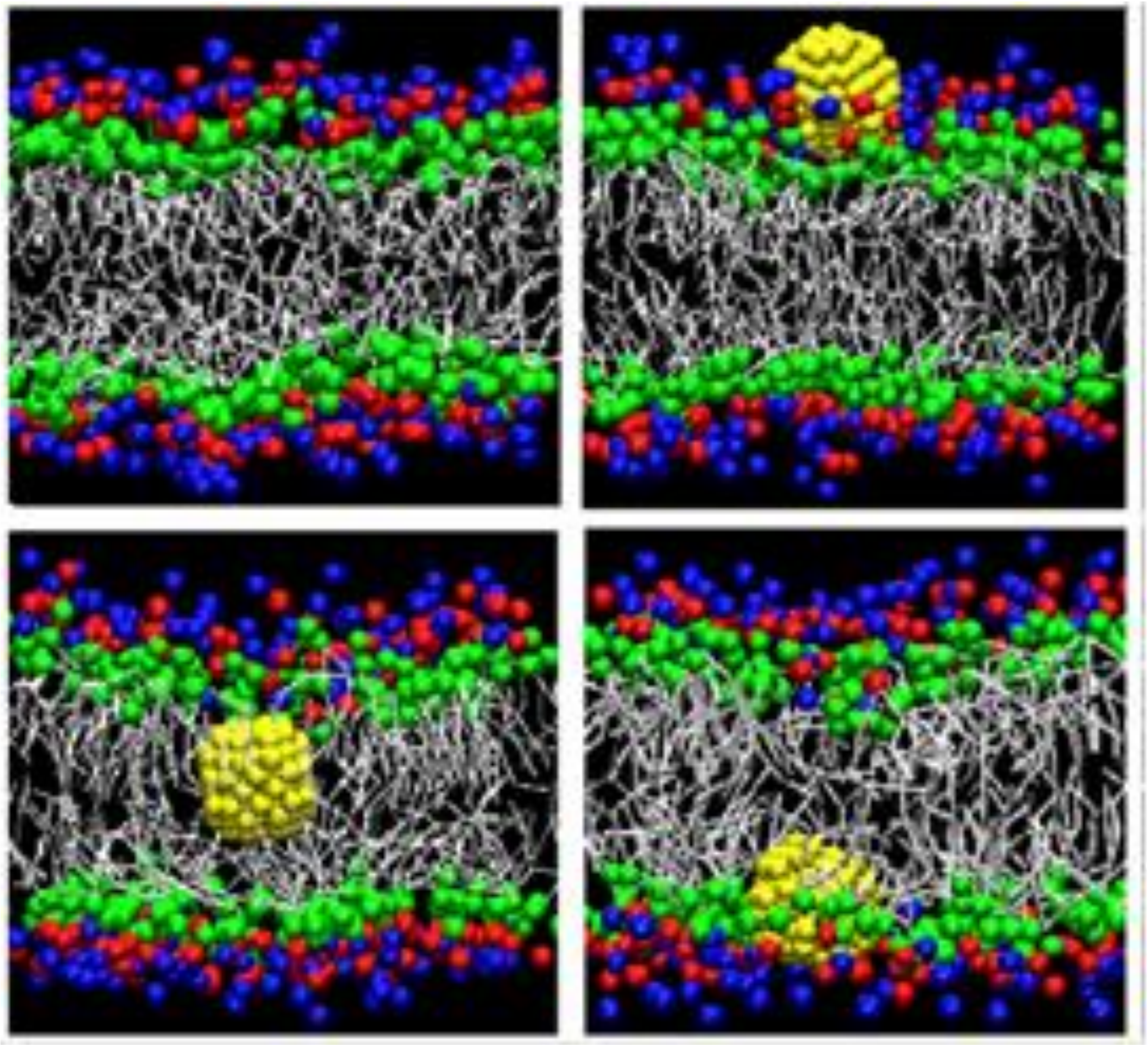
Coarse-grained mapping strategy of a DPPC lipid molecule.



The structure of gold nanocrystals (bare gold nanoparticles) with diameter of 1.0 nm, 1.5 nm and 2.0 nm.

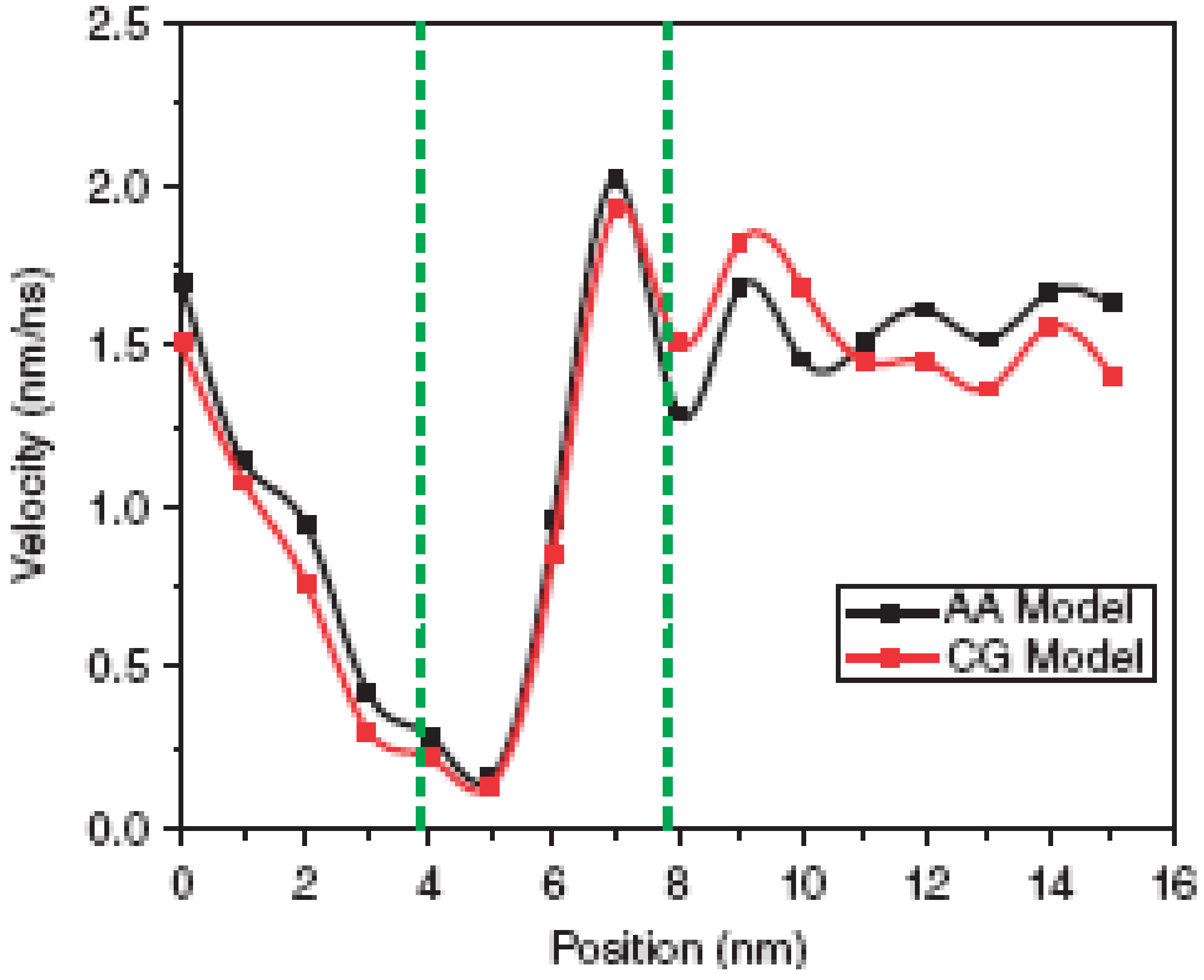


Side view of the simulation system for investigating the transport of a gold nanocrystal across the DPPC lipid membrane. (Yellow dots represent the gold nanocrystal, blue the choline group, red the phosphate group, orange the glycerol group, green the acyl chain tail group, white dots are water molecules). Gold nanocrystals, of sizes from 0.8 nm to 2.0 nm, are introduced into the water phase. A range of external forces is applied

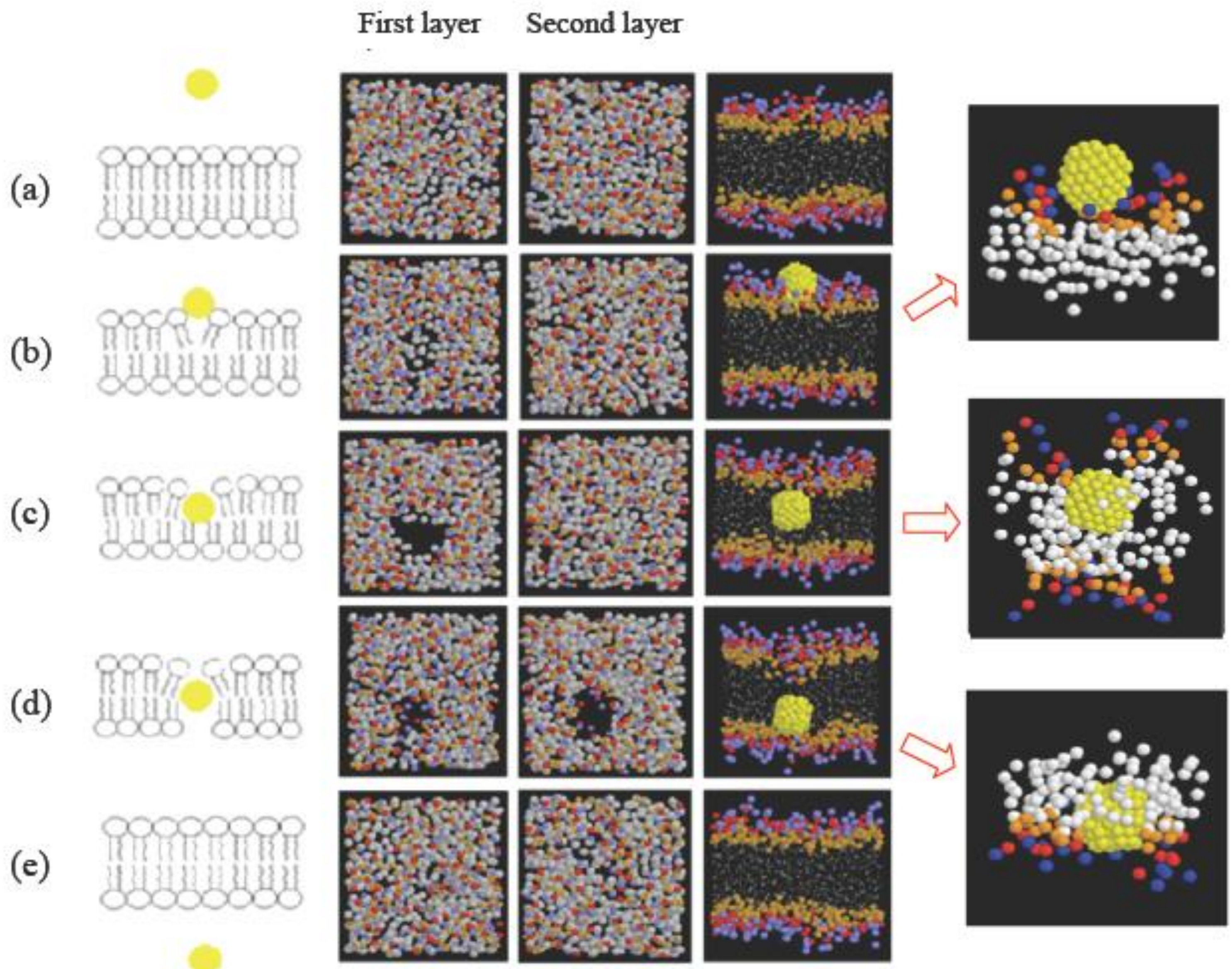


Snapshots in the permeation of the nanocrystal across the lipid membrane.

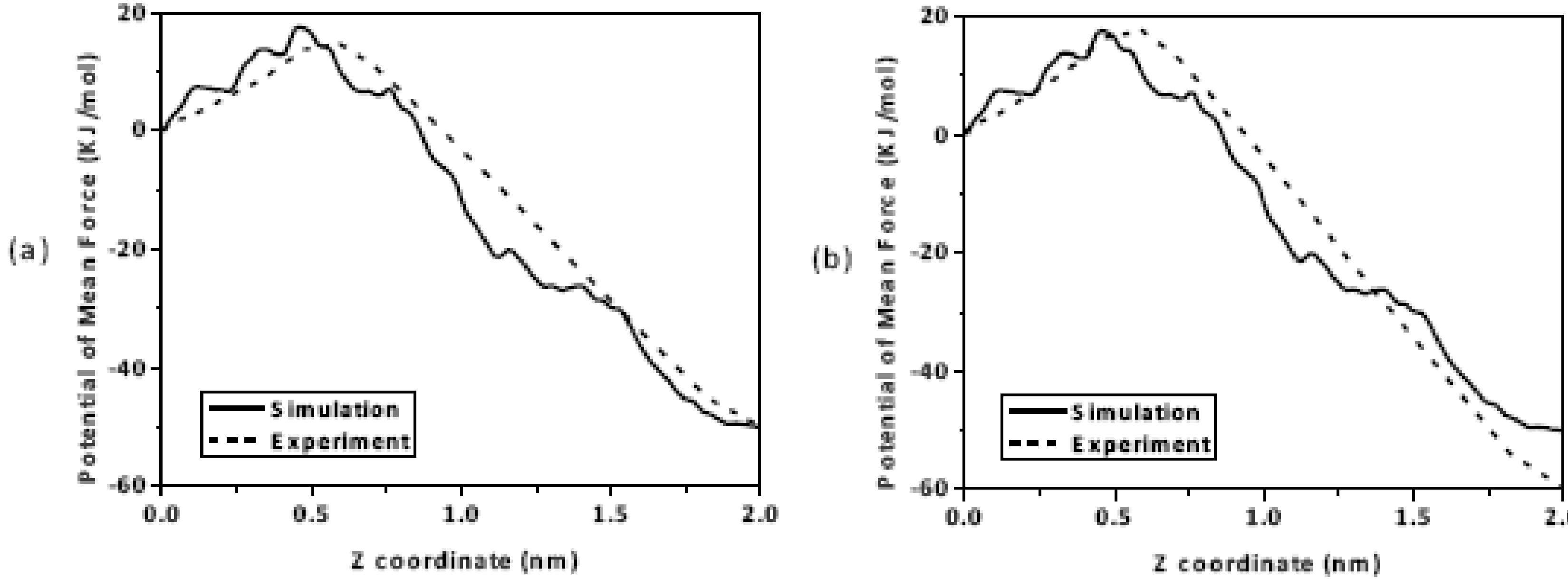
CG Model provides comparable results to All-atom Model



A comparison of velocity profiles of a nanocrystal (modelled using either an AA or CG model) permeating the lipid bilayer membrane.



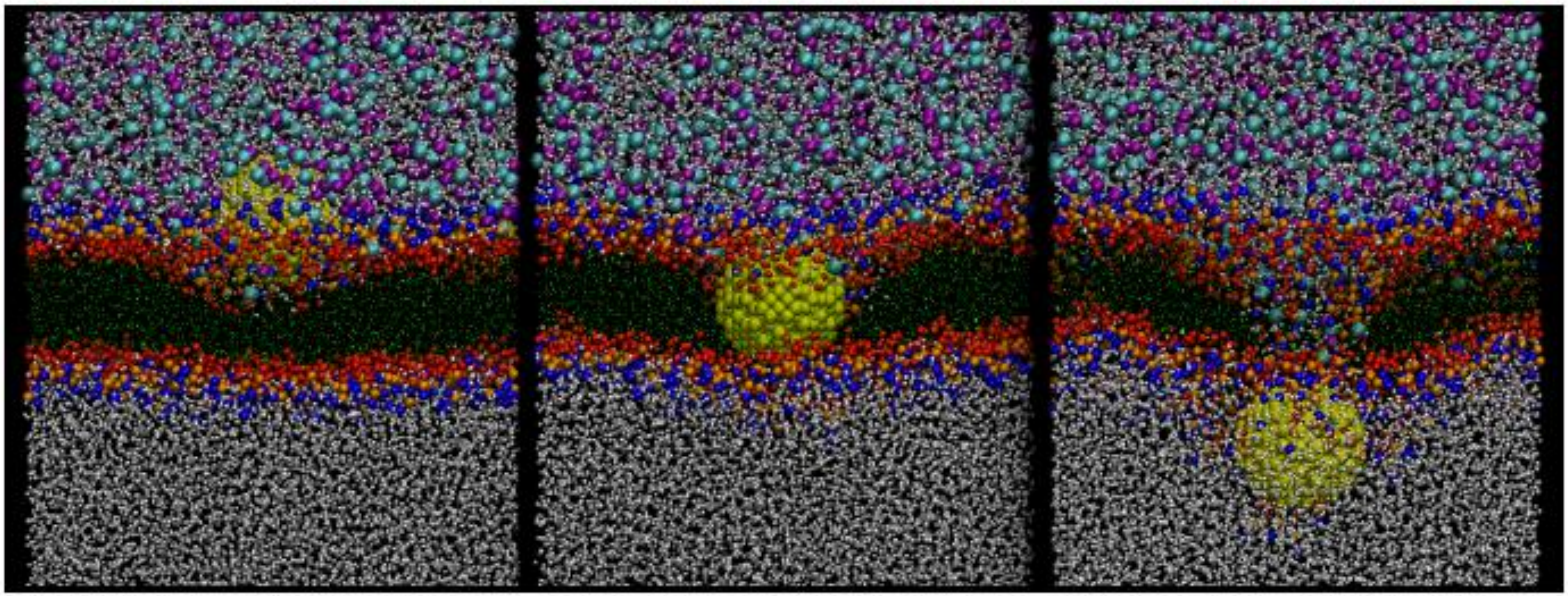
Snapshots in the permeation of the nanocrystal across the lipid membrane. The behaviors of the first and second layers of the lipid are shown. (a) the initial equilibrium configuration, (b) nanocrystal attaches to the first layer, (c) nanocrystal leaves the first layer, (d) nanocrystal attaches to the second layer, (e) nanocrystal leaves the second layer.



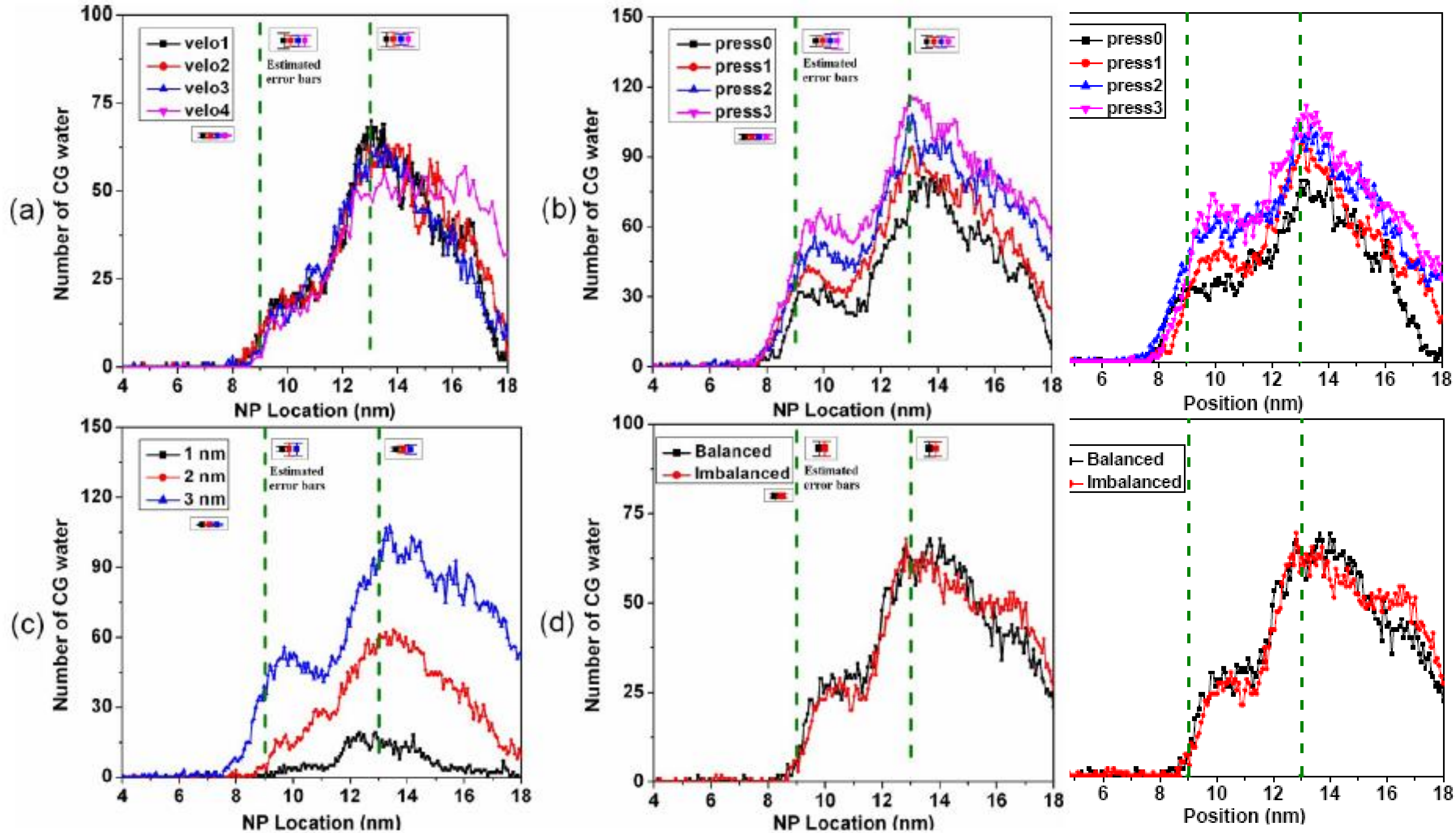
Potential of mean force profiles from simulation and experiment. Experimental value was normalized by (a) using Minimum value of PMF profile (b) using maximum value of PMF profile.

***Our force profile resembles that observed for an Au-coated nanotube tip penetrating the cell membrane in the experiments reported by** Vakarelski, I.U., et al., Penetration of living cell membranes with fortified carbon nanotube tips. Langmuir, 2007. 23(22): p. 10893-10896.*

Water permeation



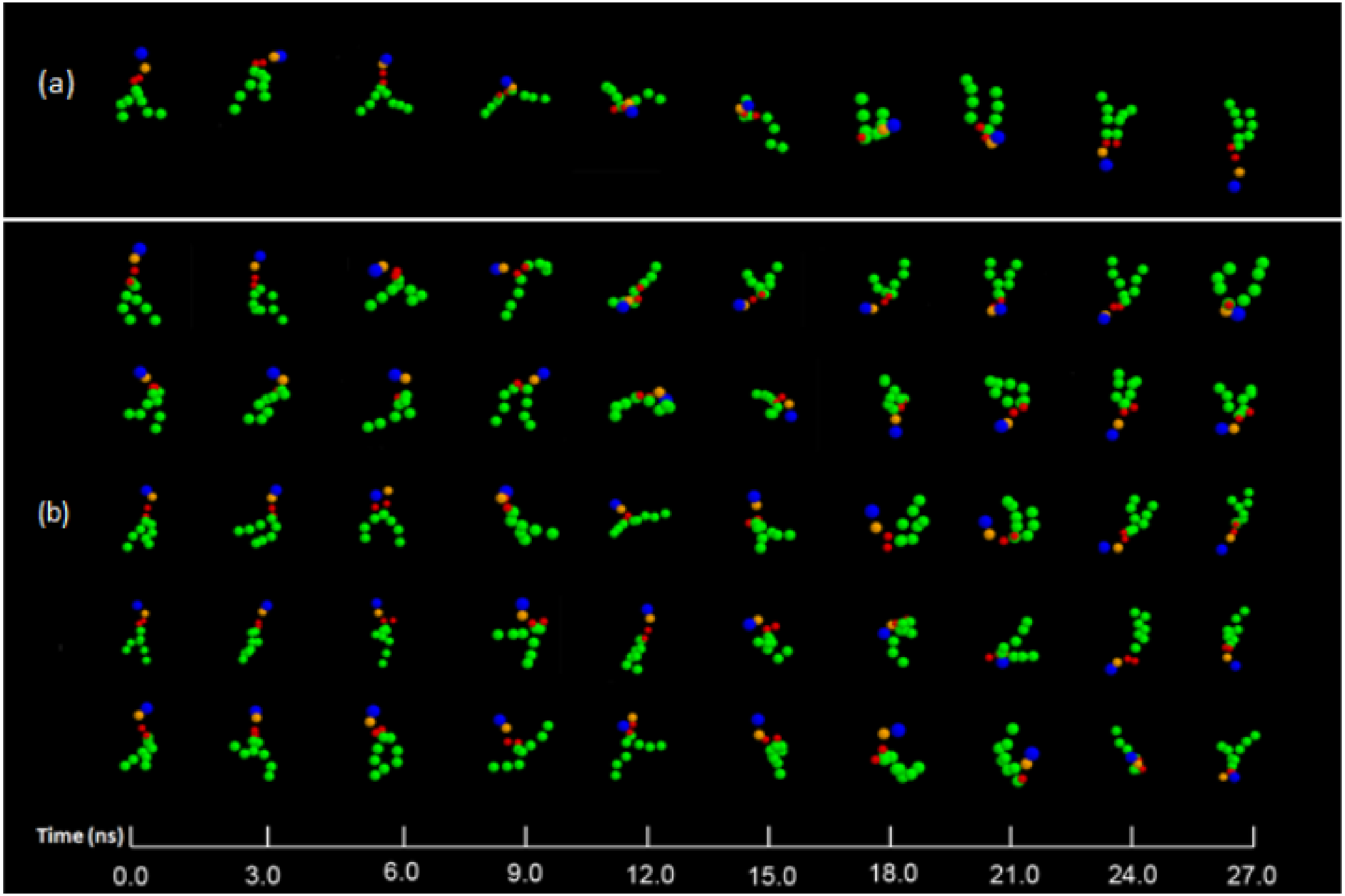
Typical snapshots for the water and ion translocation mediated by a 3.0 nm nanoparticle permeating the membrane.



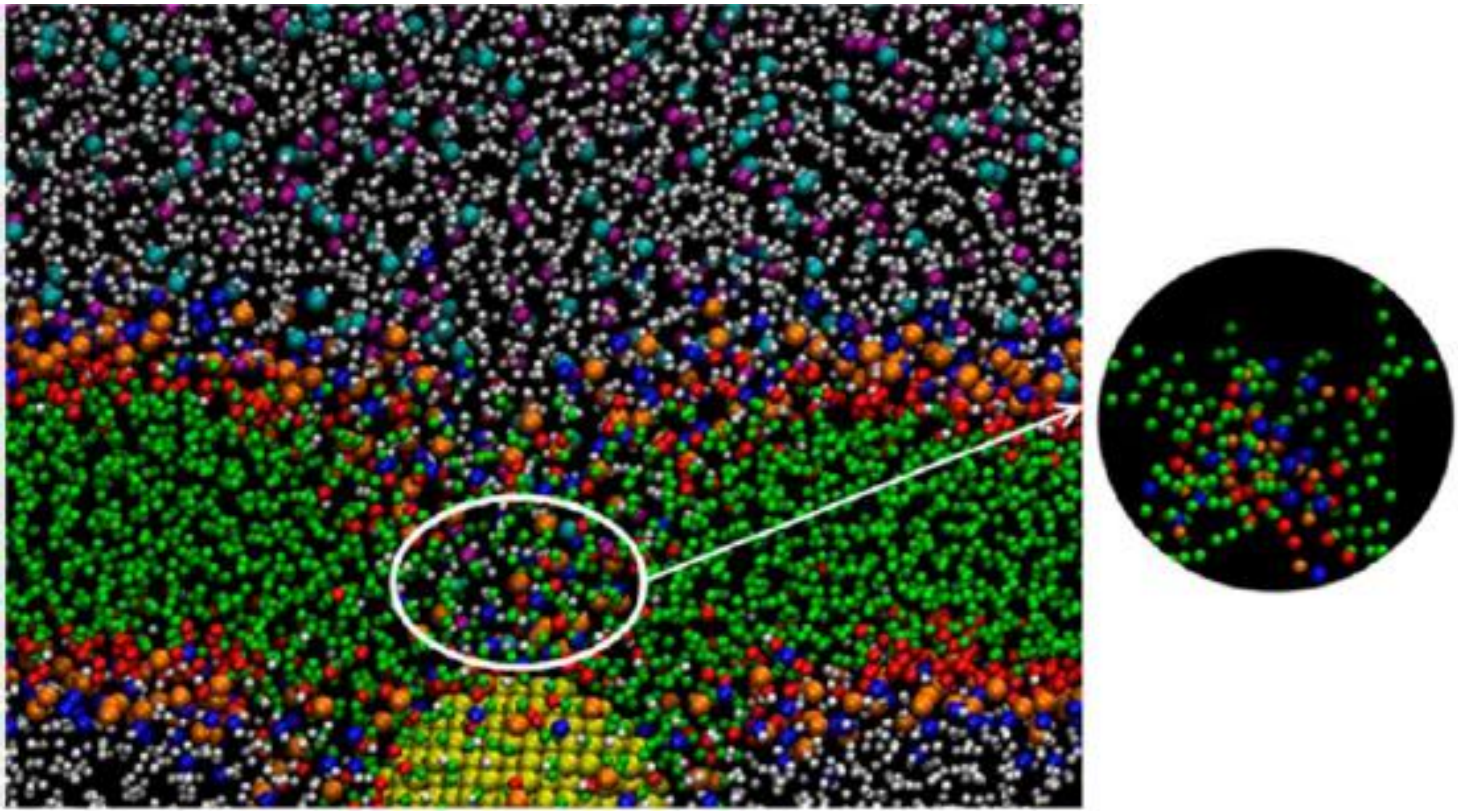
Number of water molecules in the interior of membrane under various conditions. The green dash line indicates the equilibrated position of phosphate groups (a) The nanoparticle permeation velocity effect (2.0 nm nanoparticle, balanced concentration and press1) (b) The pressure effect (3.0 nm nanoparticle, 0.7 m/s nanoparticle velocity and imbalanced ion concentration. (c) The size effect, (balanced concentration, 0.7 m/s nanoparticle velocity and press2) (d) The potential gradient effect (2.0 nm nanoparticle, 0.7 m/s nanoparticle velocity, press3.

Lipid Flip-flop events

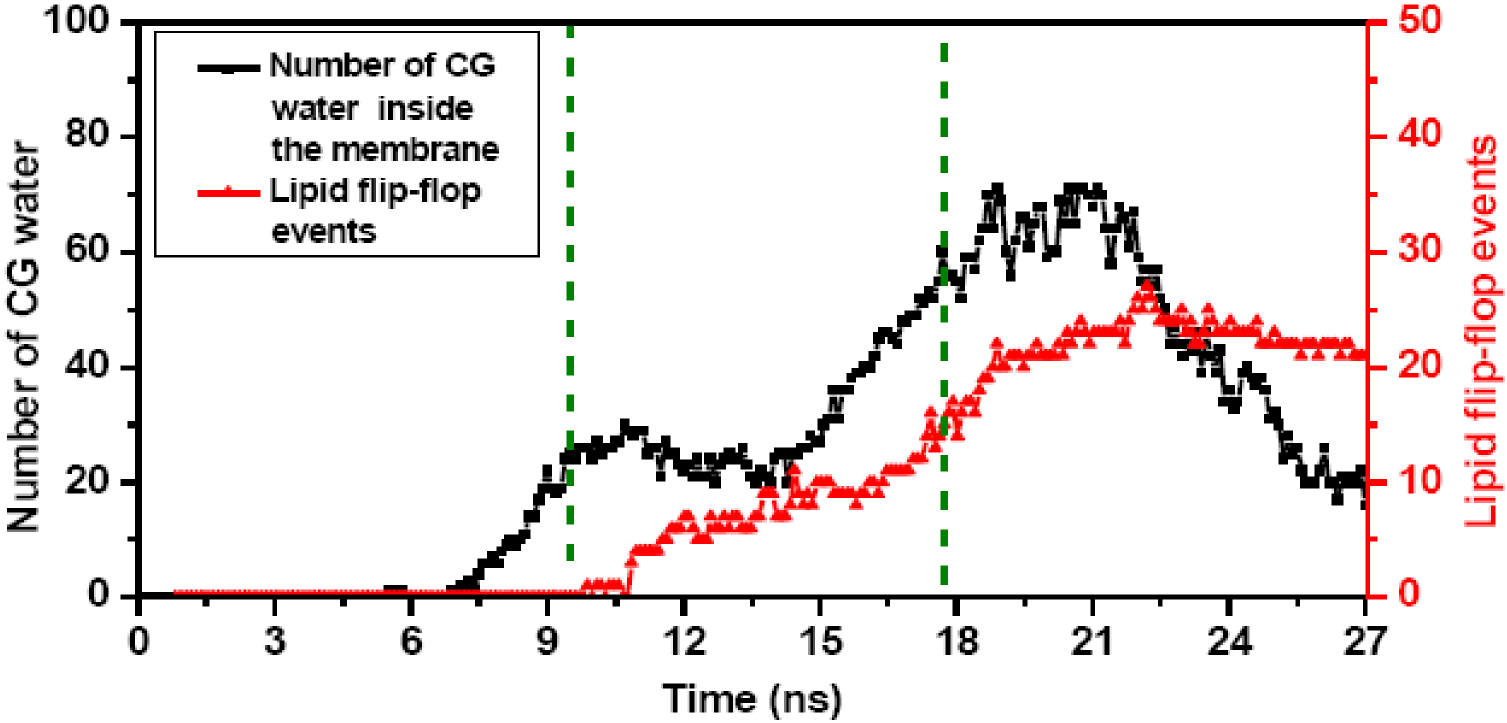
Lipid Flip-flop



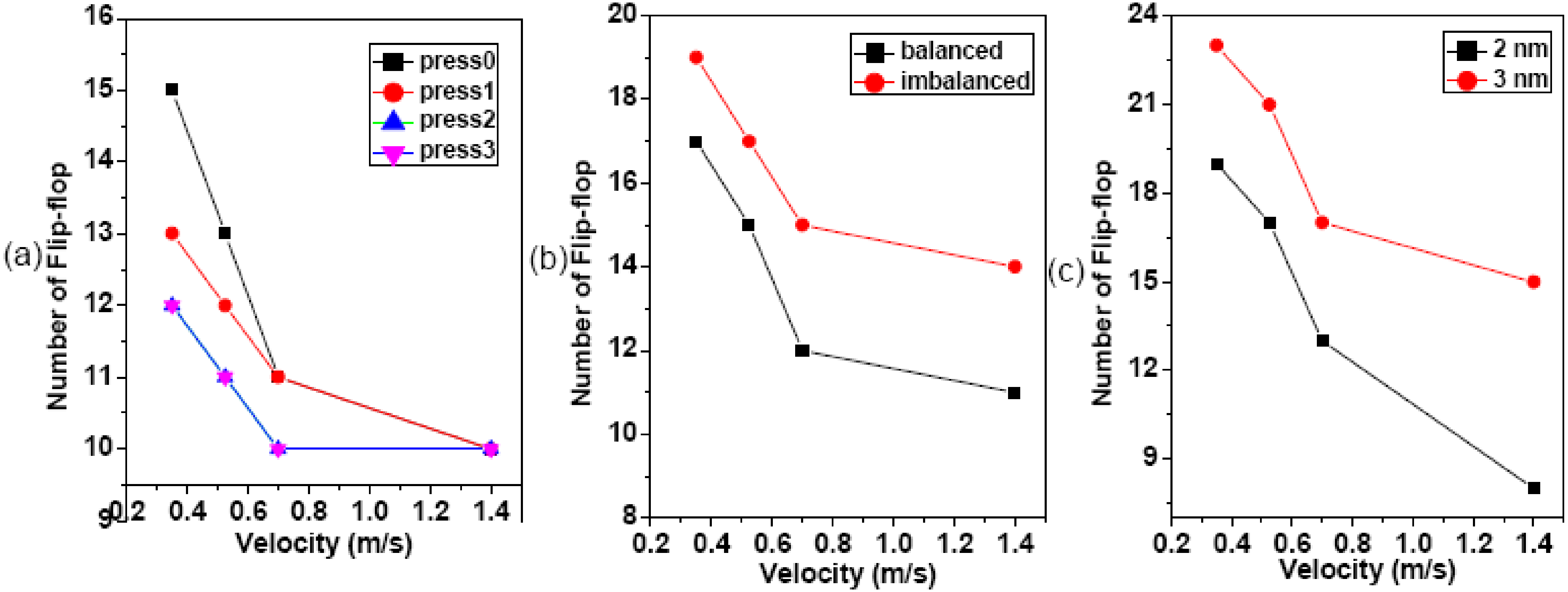
The scheme (a) and the snapshots (b) of typical lipid molecule flip-flop events observed in our simulation for a bare 3.0 nm nanoparticle permeation (0.525 m/s permeation velocity) under unequal ion concentration and press1 system.



Snapshot showing lipid molecule flip-flops as the nanoparticle is moving out of the membrane. For clarity only a section of the simulation box is shown. The inset shows only the lipid molecules in the marked region.



Number of water molecules in the interior of membrane and the instantaneous lipid molecule flip-flop events, which are obtained from 3.0 nm nanoparticle permeation (0.525 m/s permeation velocity) under unequal ion concentration and press1 system. (The green dash line indicates the time during which the center of the nanoparticle is within the membrane.)



Lipid molecule flip-flop events under various conditions.

(a) The effect of pressure differential and nanoparticle permeation velocity (2 nm nanoparticle and equal ion concentration).

(b) The effect of potential gradient (3 nm nanoparticle under press1)

(c) The effect of nanoparticle size (unequal ion concentration under press1)

Permeation of nanocrystals across lipid membranes," B. Song, H.-J. Yuan, C. J. Jameson and S. Murad, ***Mol. Phys***. <u>109</u>, 1511-1526 (2011).

Nanoparticle Permeation Induces Water Penetration, Ion Transport and Lipid Flip-Flop", B. Song, H.-J. Yuan, S. V. Pham, C. J. Jameson, and S. Murad, ***Langmuir***, <u>28</u>, 16989-17000 (2012).

Acknowledgments:

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