MOLECULAR DYNAMICS SIMULATIONS ON THE INTERACTION BETWEEN A SILVER NANOPARTICLE AND LIPID MONOLAYERS

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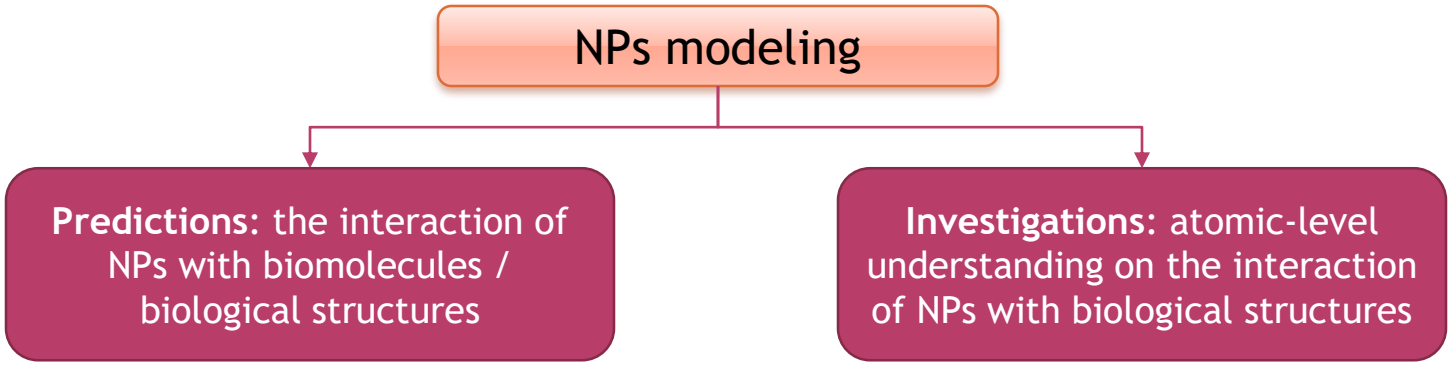
INTRODUCTION

NANOPARTICLES
1-100 nm

APLICATIONS in biomedical fields:
- -antibacterial agents
- -cancer therapy
- -drug delivery
- -biosensing
- -bioimaging
- -etc.

Potential TOXICITY!

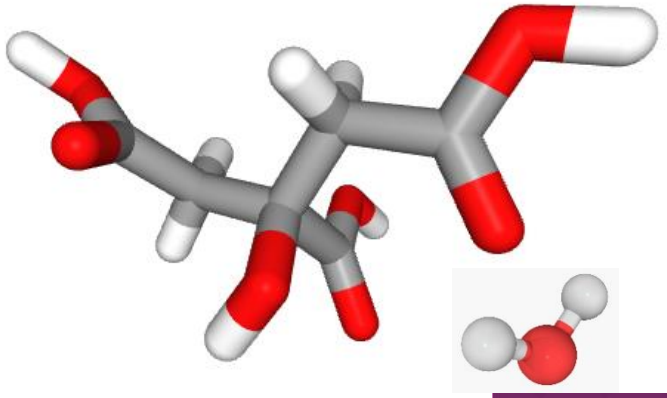
Wet-lab experiments: interaction of NPs with cells and biomolecules



DIFFICULTIES:
-**large size** – large simulation system – extensive calculations
-simulation parameters

NANOPARTICLES MODELING

$$U = U_{bonded} + U_{non-bonded}$$



$$U_{bonded} = U_{bond} + U_{angle} + U_{dihedral} + U_{improper}$$

$$U_{bond} = \sum_{bonds} K_b(b - b^0)^2$$

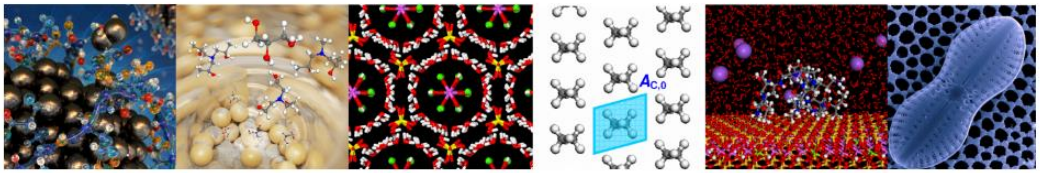
$$U_{angle} = \sum_{angles} K_\theta(\theta - \theta^0)^2$$

$$U_{dihedral} = \sum_{dihedrals} K_\varphi((1 + \cos(n\varphi - \delta))$$

$$U_{improper} = \sum_{impropers} K_\omega(\omega - \omega^0)^2$$

DESIGNING BIOLOGICAL AND NANOSTRUCTURED MATERIALS

Heinz Laboratory @ CU Boulder



overview / people / research / publications / interface md / opportunities / education / news

INTERFACE MD

https://bionanostructures.com/interface-md/

$$U_{non-bonded} = U_{LJ} + U_{elec}$$

$$U_{LJ} = \sum_{nonb.pairs} \varepsilon_{ij} \left[\left(\frac{r_{ij}^{min}}{r_{ij}} \right)^{12} - 2 \left(\frac{r_{ij}^{min}}{r_{ij}} \right)^{6} \right]$$

$$U_{elec} = \sum_{nonb.pairs} \frac{q_i q_j}{\epsilon r_{ij}}$$

Parameters for:

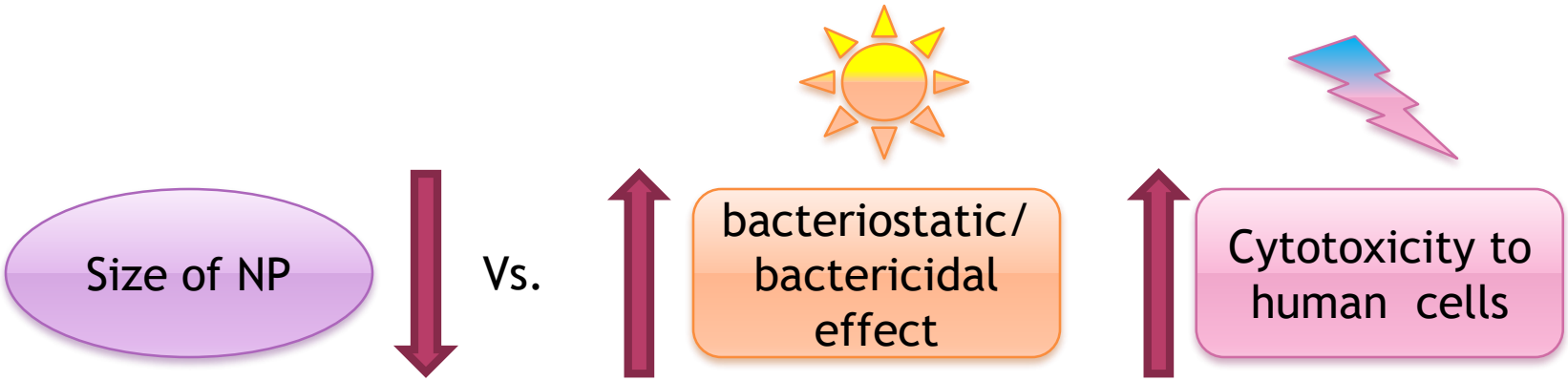
-clay / cement minerals
-metals (Ag, Al, Au, Cu, Ni, Pb, Pd, Pt)
-silica
etc.

SILVER NANOPARTICLES

-currently added to many commercial products due to their proven antimicrobial properties

-disrupt bacterial cell membranes

-also toxic for eukaryotic cells

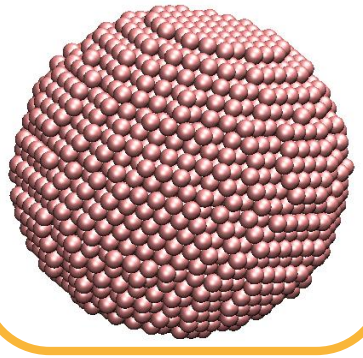


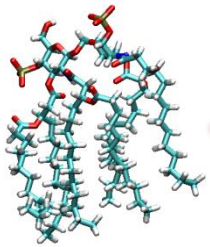
Here we used molecular dynamics to study the disruption of Gram-negative bacteria and eukaryotic cell membranes by 5 nm size Ag NPs.

METHOD

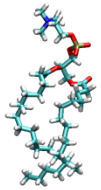
NP modeling:
CHARMM-
METAL

4302 atoms



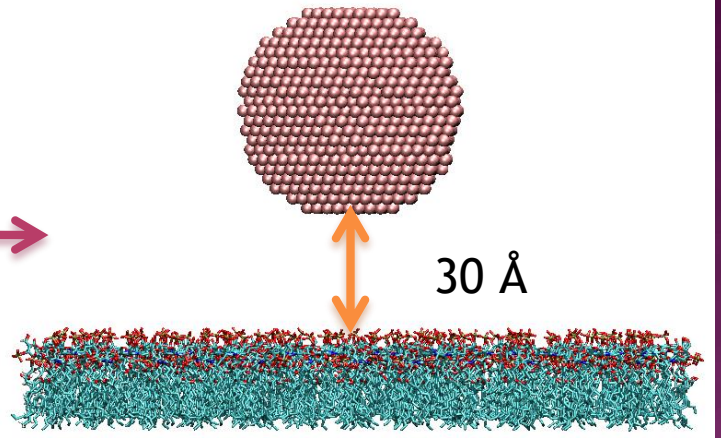


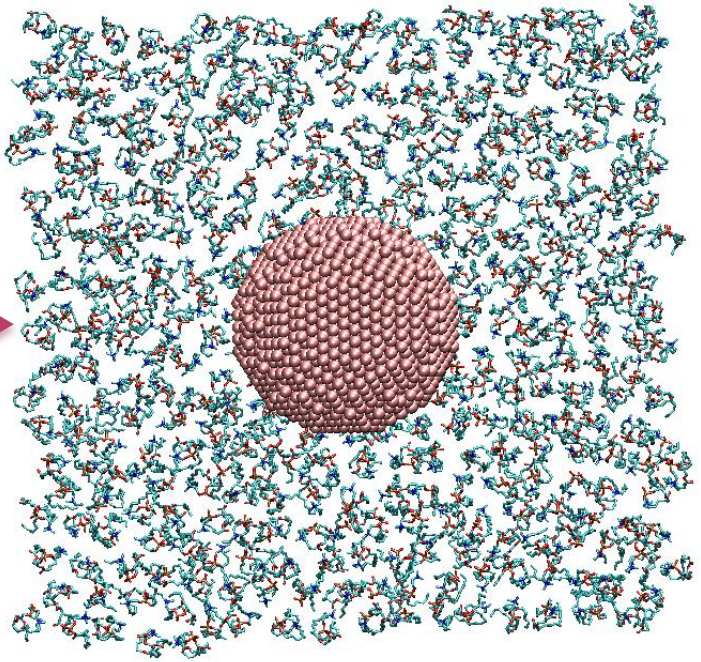
118 LPS
E. coli



356 DPPC

39348 atoms

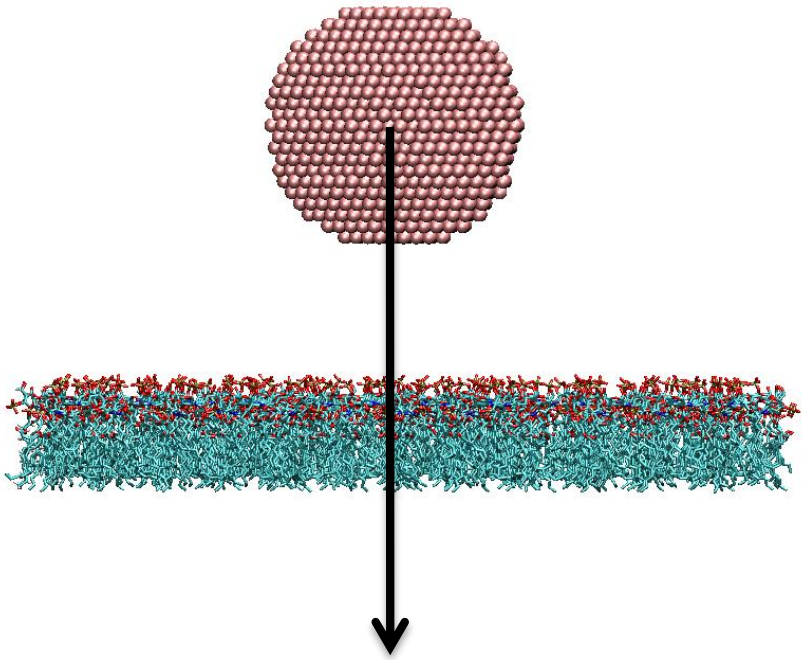




50582 atoms

METHOD

Steered Molecular Dynamics (SMD)



- Calculations with NAMD

- Velocity: 0.0002 Å / 2 fs

- 2 ns

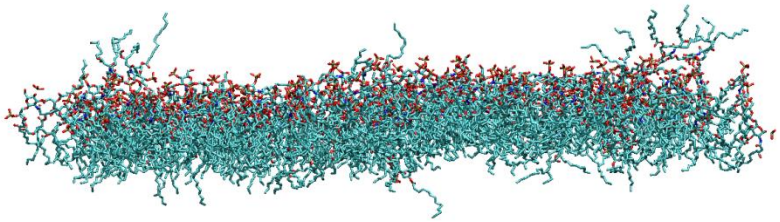
- Implicit solvent with ionic concentration 150 mM

+ control simulations: LPS and DPPC monolayers (2 ns MD)

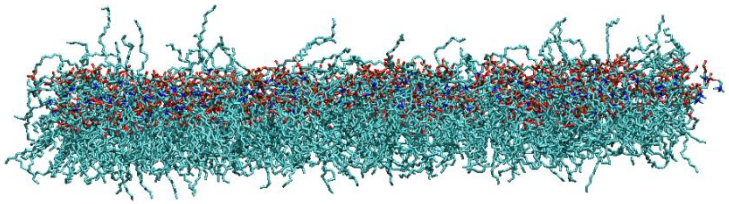
RESULTS

Control simulations

LPS

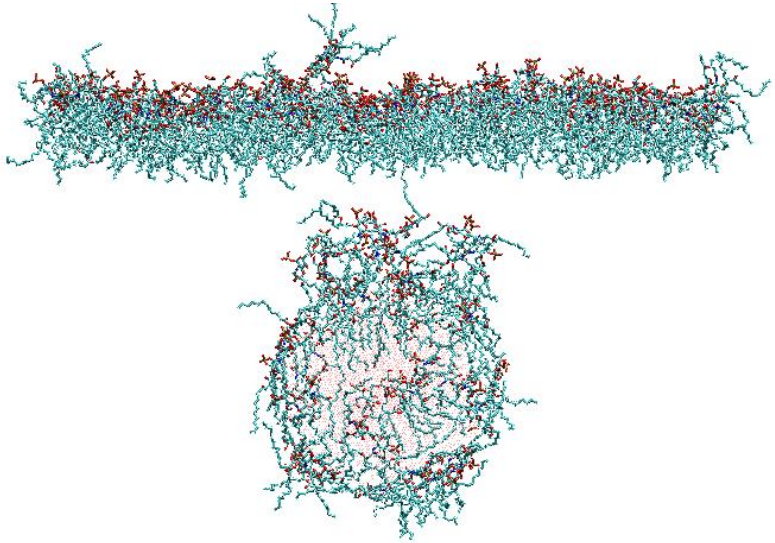


DPPC

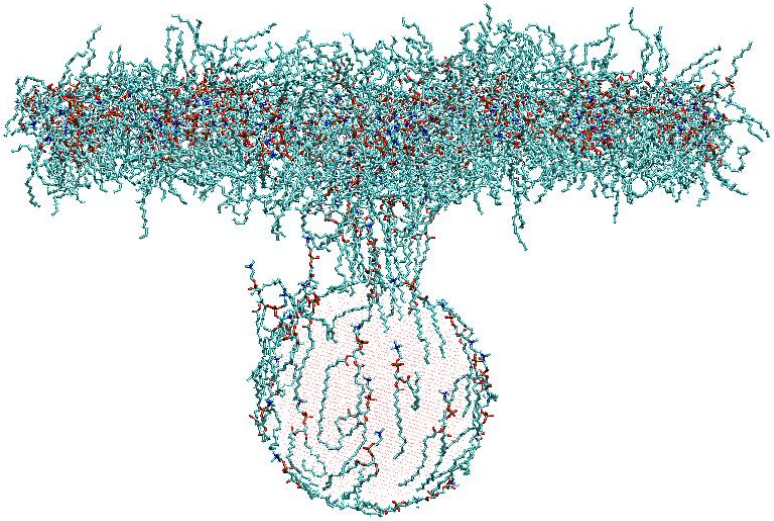


Simulations with NP

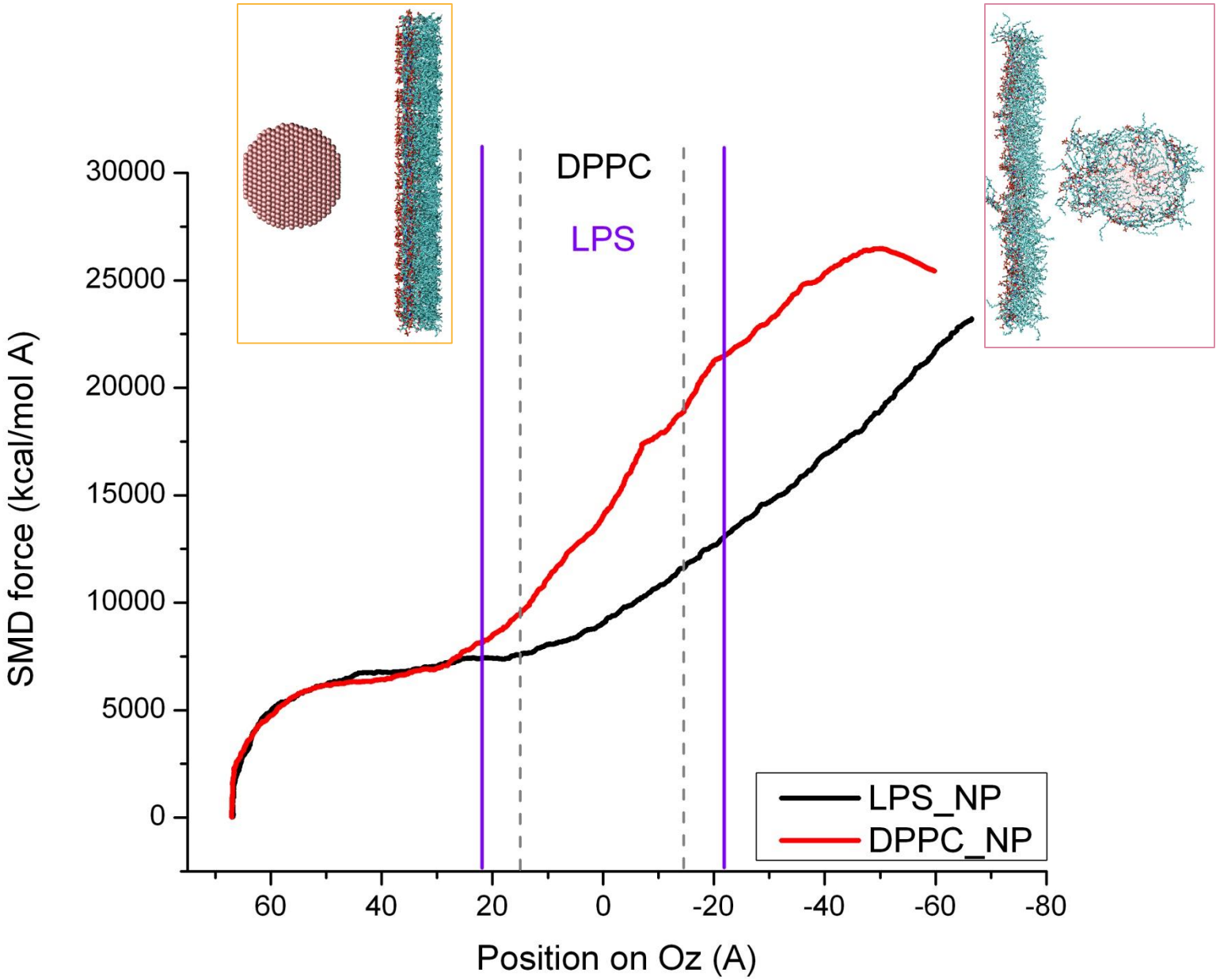
LPS



DPPC



RESULTS


DPPC
LPS
SMD force (kcal/mol A)
30000
25000
20000
15000
10000
5000
0
60
40
20
0
-20
-40
-60
-80
Position on Oz (A)
LPS_NP
DPPC_NP

CONCLUSIONS

- Simulations reveal that the LPS monolayer is more “sensitive” to the action of the NP
- Future work will focus on interpreting the data
- Perspectives:
  - the simulation of NP – bilayers interactions,
  - Simulations with explicit solvent
  - Modeling other NP and applying the methods developed here

ACKNOWLEDGEMENT

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