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Measuring Zeta Potential of High Density Lipoprotein Using Molecular Dynamics Simulations

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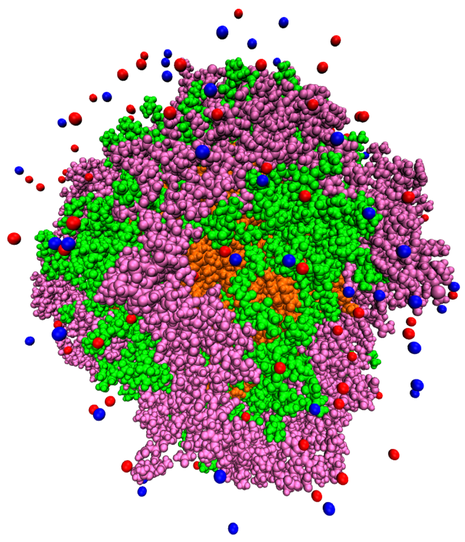
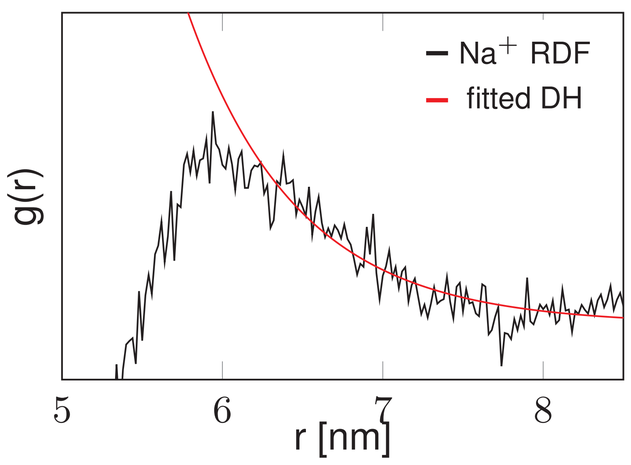
HDL

- High Density Lipoprotein (HDL) is the smallest of the five major groups of lipoproteins which play essential role in plasma lipid transport.
- HDL transports cholesterol from blood vessels to liver for excretion and it is usually called “good cholesterol”.
- We have done MD simulations of HDL in NaCl solution using OPLS-AA force field and one interesting property to be quantified is the ζ-potential.

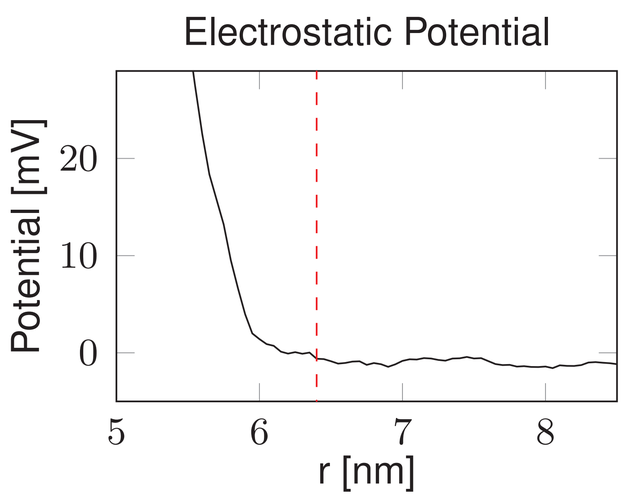


Slipping Plane

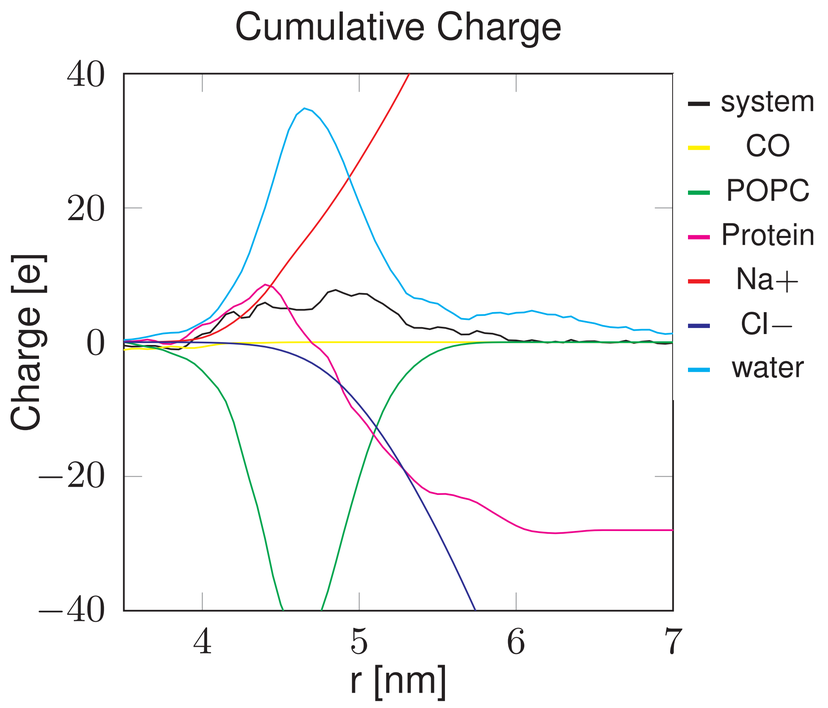
- According to Debye-Hückel theory (DH) the radial distribution of freely moving counter ions around charged particle is $Ae^{-Br}/r + C$. [1]
- When DH curve is fitted to measured distribution of counter ions (Na^+) the point where these two curves emerge is the *slipping plane*.



Electrostatic potential



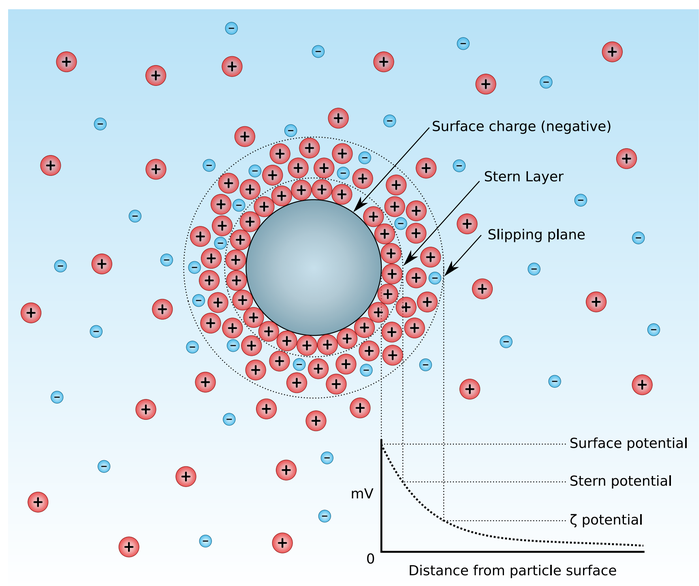
- When electrostatic potential around HDL is calculated we see that the potential on slipping plane is close to zero.
- According to experimental results the ζ-potential of HDL would be $-12,4\ mV$. [2]



- Cumulative charge of the system shows that the net charge of HDL is positive although the apolipoprotein of HDL has negative charge.

Zeta Potential

- Zeta potential (ζ-potential) is the electrical potential on the slipping plane of electrical double layer around a charged particle.



(Source: Wikipedia. Image by Larryisgood)

- The magnitude of the ζ-potential gives an indication of stability of a colloidal system.
- ζ-potential can can be determined experimentally by measuring Electrophoretic mobility.

Conclusions

- The computationally determined value of ζ-potential differs from experimentally measured value.
- Positive effective charge of HDL is probably caused by strong orientation of water molecules on the surface of the particle.
- Also too strong attraction between lipids and ions in the force field is a possible reason.

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References

[1] E. Heikkilä, A. A. Gurtovenko, H. Martinez-Seara, H. Häkkinen, I. Vattulainen, and J. Akola. Atomistic Simulations of Functional $Au_{144}(SR)_{60}$ Gold Nanoparticles in Aqueous Environment. *The J. of Phys. Chem. C*, 116:9805–9815, 2012.

[2] W.-L. Zhang, X. Gu, H. Bai, R.-H. Yang, C.-D. Dong, and J.-P. Liu. Nanostructured lipid carriers constituted from high-density lipoprotein components for delivery of a lipophilic cardiovascular drug. *International Journal of Pharmaceutics*, 391(1–2):313 – 321, 2010.