

## Classical Methods Applied to DNA-Stabilized Silver Clusters

Xi Chen, Alexander Karpenko and Olga Lopez-Acevedo

*Department of Applied Physics, Aalto University School of Science*

*xi.6.chen@aalto.fi*

DNA-stabilized metal clusters have attracted a lot of attention because of their possible biomedical and technological applications, such as nanoconductors, nanophotonics and biosensors[1-2]. Due to the big size of the systems and the important influence of the environment, this kind of systems is often beyond the ability of modern quantum mechanical simulations. Therefore, we are applying classical molecular dynamic simulations to such systems. I will present our latest results aiming to determine the structures of silver mediated DNA complexes and understand the the overall stabilisation mechanism.

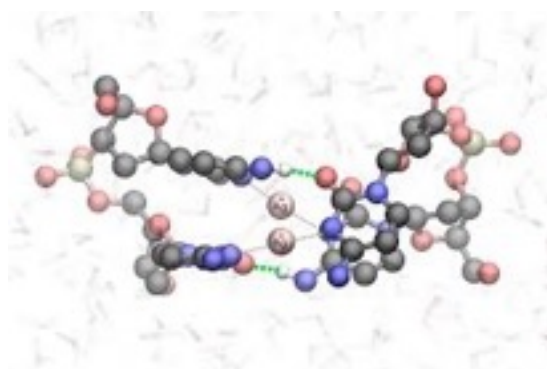


Figure 1: Silver-mediated cytosine tetramers in water. [1]

1. L. A. Espinosa Leal, A. Karpenko, S. Swasey, E. G. Gwinn, V. Rojas-Cervellera, C. Rovira, O. Lopez-Acevedo, *Journal of Physical Chemistry Letters* **6**, 4061-4066 (2015).
2. S. M. Swasey, L. Espinosa Leal, O. Lopez-Acevedo, J. Pavlovich, E. G. Gwinn, *Scientific Reports* **5**, 1-9 (2015).