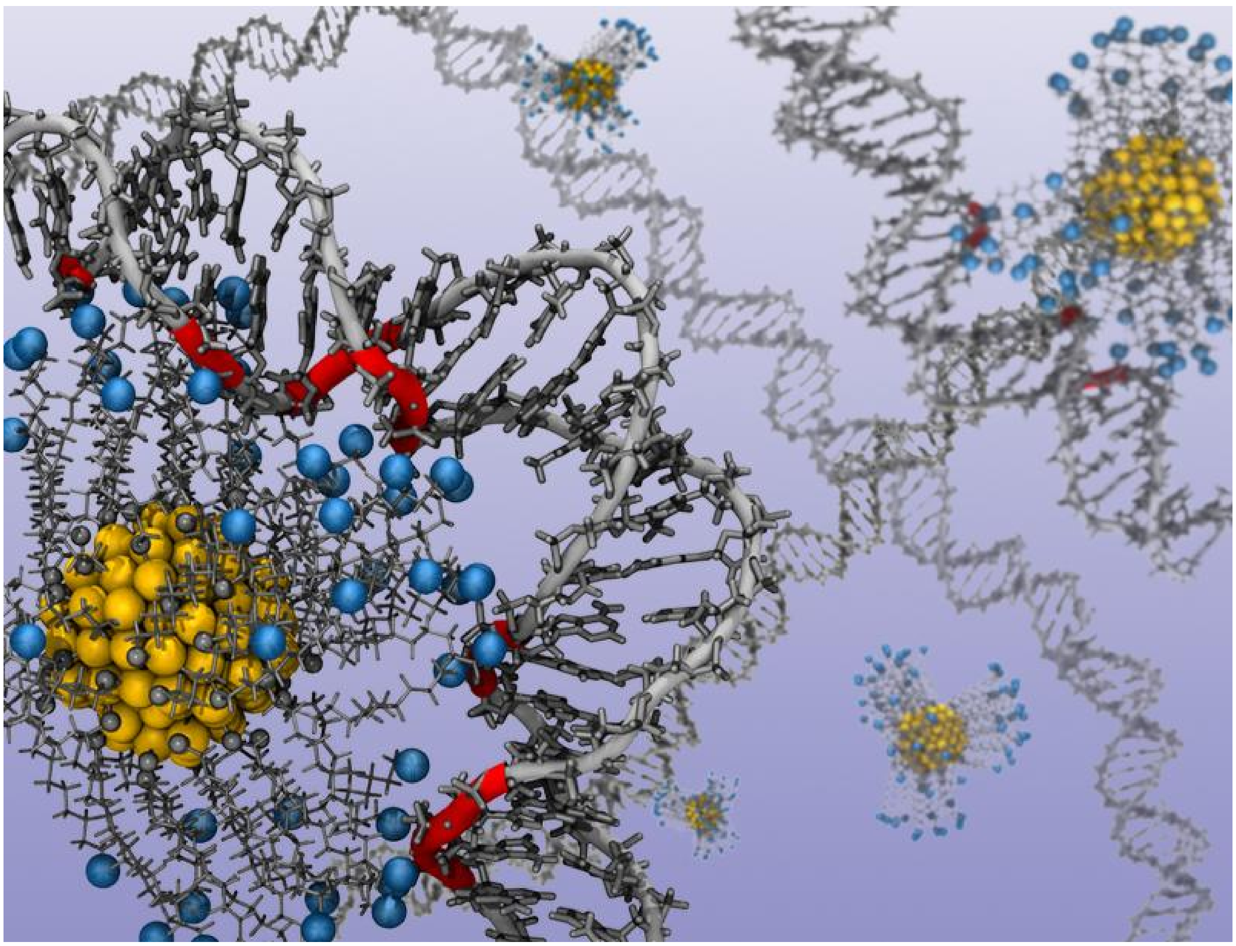
Researchers detail how to control shape, structure of DNA and RNA

November 11 2015, by Matt Shipman



Researchers used a computer model of gold nanoparticles and ligands to determine how nucleic acids respond to various charges. In technical language, the image shows the binding of alkyl ligand functionalized gold nanoparticles with protonated amine end groups (the blue spheres) to double stranded DNA. Credit: Jessica Nash

Researchers at North Carolina State University have used computational modelling to shed light on precisely how charged gold nanoparticles influence the structure of DNA and RNA – which may lead to new techniques for manipulating these genetic materials.

The work holds promise for developing applications that can store and transport genetic information, create custom scaffolds for bioelectronics and create new drug delivery technologies.

"In nature, meters of DNA are packed tightly into every living cell," says Jessica Nash, a Ph.D. student at NC State and lead author of a paper on the work. "This is possible because the DNA is wrapped tightly around a positively charged protein called a histone. We'd like to be able to shape DNA using a similar approach that replaces the histone with a charged gold nanoparticle. So we used computational techniques to determine exactly how different charges influence the curvature of nucleic acids – DNA and RNA."

In their model, the researchers manipulated the charge of the gold nanoparticles by adding or removing positively charged ligands – organic molecules attached to the surface of the nanoparticle. This allowed them to determine how the nucleic acid responded to each level of charge. An animation of a nanoparticle and ligands shaping a strand of DNA is available at www.youtube.com/watch?v=kNpvPy … bmc&feature=youtu.be.

"This will let researchers know what to expect – how much charge they need in order to get the desired curvature in the nucleic acid," says Yaroslava Yingling, an associate professor of materials science and engineering at NC State and corresponding author of the paper.

"We used ligands in the model, but there are other ways to manipulate the charge of the nanoparticles," says Abhishek Singh, a postdoctoral researcher at NC State and co-author of the paper. "For example, if the nanoparticles and nucleic acid are in solution, you can change the charge by changing the pH of the solution."

The work is also significant because it highlights how far computational research has come in materials science.

"Our large-scale models account for every atom involved in the process," says Nan Li, a Ph.D. student at NC State and co-author of the paper. "This is an example of how we can use advanced computational hardware, such as the GPUs – or graphics processing units – developed for use in videogames, to conduct state-of-the-art scientific simulations."

The research team is now building on these findings to design new nanoparticles with different shapes and surface chemistries to get even more control over the shape and structure of nucleic acids.

"No one has come close to matching nature's efficiency when it comes to wrapping and unwrapping nucleic acids," Yingling says. "We're trying to advance our understanding of precisely how that works."

More information: Jessica A. Nash et al. Characterization of Nucleic Acid Compaction with Histone-Mimic Nanoparticles through All-Atom Molecular Dynamics, *ACS Nano* (2015). DOI: 10.1021/acsnano.5b05684

Provided by North Carolina State University