

## **How does zinc enhance DNA conductivity?**

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One way to enhance the conductivity of DNA is to embed it with metal ions. Lee has shown that divalent metal ions (2+ charged atoms) can bind in-between the base-pairs in DNA, thereby enhancing its electrical properties.

I have conducted a molecular modeling study to find the geometry, energy and motion of poly-ZnGC (a DNA double-helix with metallized GC nucleotides). High-level Density Functional Theory (DFT) methods were used to calculate the optimized geometries and harmonic frequencies of a model Zn-GC base pairs. These calculations serve three purposes: 1) showing how zinc interacts with a single DNA base pair in a detailed, quantitative way, 2) explaining if the proposed models of metallized DNA are consistent with the observed electrical properties of B-DNA and Zn-DNA, and 3) helping to gain enough information about the model Zn-GC structure to re-parameterize the AMBER force field for nucleic acids so that it can also model metallized nucleic acids.

This information enables us to extrapolate from single base-pairs to an entire solvated DNA double helix using efficient, classical mechanics methods. This layered approach leads to a detailed understanding of how DNA interacts with metals and predicts important energetic properties that are crucial for engineering DNA for molecular electronics.

Below: Zn-DNA double helix with hydroxides.



