Contribution ID: **4** Type: **not specified**

Quantum-chemical modeling of mono- and biligand complexes of silver ions with some DNA nucleotide bases

Thursday, 19 March 2026 12:30 (30 minutes)

One of the promising objects for the creation of new functional materials is the metallized DNA molecule. Such a system is a unique combination of the biopolymer matrix of DNA and the properties of metal ions, in particular Ag⁺. The presence of intercalated Ag⁺ ions in the DNA structure provides the possibility of forming one-dimensional nanostructures in the form of nanowires [1]. At the same time, for the correct modeling of such systems, a necessary procedure is a step-by-step optimization, the initial stage of which is the quantum-chemical modeling of complexes of DNA nucleotide bases with Ag⁺ ions in the form of L–Ag⁺ and L–Ag⁺–L, where L is the ligands of the studied nitrogenous bases. In our case, the anions of thymine (T[–]) and guanine (G[–]), and the molecular forms guanine (G), cytosine (C), 5-bromocytosine (C-Br) and adenine (A).
Calculations were performed within the framework of density functional theory (DFT) in the Gaussian 03 software package. Argentum atoms were described by the Def2-TZVP ECP basis set. The 6-311++G(d, p) basis set was used to describe the nucleotide base atoms. The PCM and SMD models were used as solvation models. The empirical correction for the dispersion interaction GD3 was used. Calculations of the effective charge of the central atom were made using the natural orbital theory (NBO). The criterion for comparing the stability of the complexes was the energy effect of complex formation. Calculations of the energy effects of Gibbs energy, enthalpy and zero-order energy for the [Ag⁺–L] complexes were performed according to the equation:
<pre>
L + Ag⁺ = [Ag⁺–L] + ΔE₁
ΔE₁ = E(Ag⁺–L) – (E(L) + E(Ag⁺))
</pre>

For the [L–Ag⁺–L] complexes, the energy effects of formation were calculated according to the equation:
<pre>
L + [Ag⁺–L] = [L–Ag⁺–L] + ΔE₂
ΔE₂ = E(L–Ag⁺–L) – (E(L) + E(Ag⁺–L))
</pre>

It was shown that electroneutral Ag⁺ complexes with the N3 atom of thymine and the N1 atom of guanine demonstrated the highest thermodynamic stability. Positively charged complexes gave lower thermodynamic stability. Among them, Ag⁺ complexes with the N1 atom of adenine were found to be the least stable, which explains the experimentally observed "jumping out" of adenine from the double helix in the metallized Ag-DNA molecule [1]. A comparison of the computational approaches used in [2] shows that the B3LYP functional in combination with the SMD solvation model provides the most suitable description of the [Ag⁺–L] complexes, since it systematically gives lower formation energies than B3LYP/PCM and predicts the Ag-N bond lengths more consistently than M06-2X. Therefore, optimization was performed for the [L–Ag⁺–L] complexes using this method.

 Kondo, J., Tada, Y., Dairaku, T., Hattori, Y., Saneyoshi, H., Ono, A., Tanaka, Y. (2017). A metallo-DNA nanowire with uninterrupted one-dimensional silver array. Nature chemistry, 9(10), 956–960. Ye.

Osokin, S. Perepelytsya. (2026). Stability of Ag-DNA Nucleotide Base Complexes: A Quantum-Chemical Study. Low Temperature Physics, 2026, Vol. 52.

Primary authors: Dr OSOKIN, Yevhen (Bogolyubov Institute for Theoretical Physics); Dr PEREPELYTSYA, Sergiy (Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine)

Presenter: Dr OSOKIN, Yevhen (Bogolyubov Institute for Theoretical Physics)