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REGULAR ARTICLE

Charge transfer between DNA and proteins in the nucleosomes

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Abstract Recently X-ray diffraction provided the structure of nucleosomes. External disturbances can unwrap DNA from the histone–protein and their genetic information becomes readable. This is strongly connected with cancer initiation. Therefore, first we performed charge transfer (CT) calculations between polythymidine and a periodic model-protein chain with a lysine or arginine and three glycines. The CT calculations were repeated between the infinite chains using combined solid state physical and quantum chemical methods. We found that the CT between the unit cells of an infinite polythymidine and poly(lysine-triglycine) is 0.04 *e* and 0.03 *e* for poly(arginine-triglycine). We investigated the influence of the basis set quality on the calculated CT values using a molecular model built of a thymidine and lysine or arginine. We have calculated also the bands of polythymidine and the two protein model chains. We have found that the differences between the highest level of the valence band of single polythymidine chain and the lowest level of the conduction bands of the model protein chains (6-11 eV depending on the basis set) are too large to assume a direct CT between these two bands.

Keywords Nucleosome structure · Charge transfer between PO_4^-–Lys^+ · Charge transfer between PO_4^-–Arg^+ · Band structure of poly[Lys–triglycine] · Band structure of poly[Arg–triglycine]

1 Introduction

Recently the structure of the nucleosome has been determined using high-resolution X-ray diffraction measurements [1, 2]. It has been found that one nucleosome contains eight nucleohistone molecules [nucleosome core particle (NCP)] [1]. The histones are wrapped around by a 147 base pair long DNA B superhelix [2]. It is left handed and has 1.67 turns. This complicated packing of DNA makes it possible that in the nucleus of a single eukaryotic cell a 3.5 km long DNA chain can be accommodated.

At high resolution (2.8 Å for NCP and 1.9 Å for DNA) it has turned out that in contrast to an ideal DNA B superhelix, in the nucleosomes DNA is not bent uniformly. This is caused by the anisotropic flexibility of DNA, local structural deviations from the ideal form, etc. [2]. Most probably, these features (irregular bending and twisting) of the DNA superhelix which cause excess DNA curvatures are the reason that NCPs can "slide" along the DNA molecule without relaxing it [3]. The structure of the nucleosome is held together through the H-bonds of the PO_4^- groups of DNA and the positively charged lysine (*lys*) and arginine (*arg*) side chains of the histones (they are rich in them) as well their other H-bond donor sites (like serine,

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threonine, etc.). As subsequent investigations have shown, there are 120 possibilities of H-bond formation between DNA and the proteins in one nucleosome [4]. This makes it possible to estimate the positive charge per base on DNA and the negative charge on the histone side chains (taking the other positive sites in the histones as side chains). Because of the charge transfers (CTs) one would expect a positive hole current (due to local electric fields) in DNA and a negative electronic one through the histones.

In [1] and [2] it is pointed out also that if something (binding of foreign chemicals, radiation, etc.) changes the relative conformations of the histones and DNA, a part of the DNA chain will unwrap. In this way the H-bonds will break and with them, of course, the CT of the unwrapped section will disappear. This diminishes or interrupts the positive and negative currents, respectively. This procedure can happen through several nucleosomes. Namely, also the structure of a tetranucleosome was determined at 1.9 Å resolution [5] and on the basis of it a chromatin model was developed [6]. In this model two stacks of nucleosomes starting in opposite directions are presented [6].

Most probably, this chain of events may occur in a chromatin simultaneously at many places. In this way many genes of DNA become freely readable at an unexpected time point. Most probably there are a certain number of genes among them which take part in the self-regulation of the cell (among the 50,000 genes of a cell 5,000 have some regulatory function [7]). This leads through biochemically and mechanically well-known processes (transcription to mRNA and translation to proteins) to the occurrence of a number of oncoproteins at a point in a time and at specific locations where they were not expected to be present. It is easy to imagine that all these events disturb the self-regulation of the cell. A part of these cells could be in new stationary states, which are precancerous [8, 9].

To understand better the details of the phenomena inside the nucleosomes, we have started a series of rather large-scale quantum theoretical investigations, applying solid-state physical methods for infinite chains. First we have computed the Hartree–Fock (HF) band structures [10, 11] for all the four periodic homopolynucleotides: poly(adenilic acid), poly(guanilic acid), polythymidine and polycytidine in the presence of water and Na^+ ions using the crystal orbital (CO) [10] method in the case of combined symmetry operation [11]. For details regarding the methods, see [10, 12]. We have obtained band structures at which nucleotide base-type valence and conduction bands occur with fundamental gap values of 11–12 eV. There are no bands in the neighborhood of the valence bands, but there are a larger number of non-nucleotide base-type empty bands (sugar-, phosphate-, Na^+ ion- and water-type bands in the gap near to the conduction band). This situation excludes the possibility of electronic-type doping in DNA.

The valence bands of three homopolynucleotides (but not of the polycytidine) are broad enough that Bloch-type conduction can take place in them if they are doped by electron acceptors. They are more than ten times broader than the thermal energy at 300 K, $k_B T = 0.025$ eV, where k_B is the Boltzmann constant and T the temperature in Kelvin. Due to the CT between the PO_4^- groups of DNA and the lys^+ and arg^+ side chains of the nucleohistones, one would expect a hole-type positive current in DNA. This is in accordance with the experimental findings of Porath et al. [13, 14] who measured I–V characteristics (I being the electrical current and the V the voltage) of a short DNA chain in contact with two metal electrodes. Similar measurements were carried out recently by Guo et al. [15] with a DNA duplex bridging a carbon nanotube gap. The purpose of our CT calculations between DNA and proteins is to calculate the conductivity of the biological macromolecules.

In two previous papers [16, 17] we have calculated CT between the PO_4^- groups of DNA and the lys^+ and arg^+ side chains, respectively, of the histones. In the first paper, we have not taken into account the screening effect of water molecules and a K^+, and in this way we have obtained unrealistically large CT values.

In the second paper, we have applied the two-layer ONIOM method [18–20]. Here the water molecules, the K^+ ion and the PO_4^- group as well as the lys^+ and arg^+ side chains of the histones formed the *model* system, while in the *real* (supermolecular system) in addition, also the deoxyribose part of DNA and a thymine molecule was added. The *real* system was treated by the simple HF method with 6-31G basis set, while for the *model* system both HF and second order Møller–Plesset (MP2) perturbation theory were applied using Ahlrichs' basis set with polarization functions (TZVP) [21] for the geometry optimization. In this way we were able to exclude the spatial coincidence of the positions of the water molecules or the K^+ ion with the DNA constituents which might occur if only the model system is considered. For the population analysis we have used besides Mulliken method [22] also the natural bonding orbital (NBO) method [23, 24]. As basis sets for the population analysis, either Clementi's double ξ basis set [25] or the already-mentioned TZVP basis set [21] was applied. For the geometry optimization of the *model* system (see before) the TZVP basis set with the MP2 (with counterpoise correction) method was applied [17], while for the rest of the *real* supermolecular system (sugar + thymine) Olson's geometry [26] was used.

It is well known that in the TCNQ (tetracyanochinone)–TTF (tetrathiofulvalene) system there is 0.6 e CT from

TTF to TCNQ [27], while there is no CT between a single TTF and TCNQ molecule pair [28]. For this reason we have calculated also the CT between a thymine (T)–sugar (S) and PO_4^- chain and a chain built up from either *lys* or *arg* and glycine (*gly*) molecules (see Fig. 1). (It should be pointed out, however, that the TCNQ-TTF system forms a three-dimensional crystal and at certain symmetry points the valence and conduction bands cross each other).

Since the amount of the charge transferred from DNA to the histones is not at all trivial, the simple molecular view (investigation of a nucleotide and amino acid) may be misleading as has occurred in the previously mentioned TCNQ–TTF case. In this paper, we report the results obtained from the infinite chain calculation. This model preserves the most important features of the DNA–protein interaction in the real nucleosome and provides an insight into the possible solid-state physical effects on this interaction as well as on the CT, which is the main topic of this paper.

2 Methods

The calculation of CT for the nucleosome is a formidable computational task. Therefore, we need to build a model with simplifications that preserves the most important

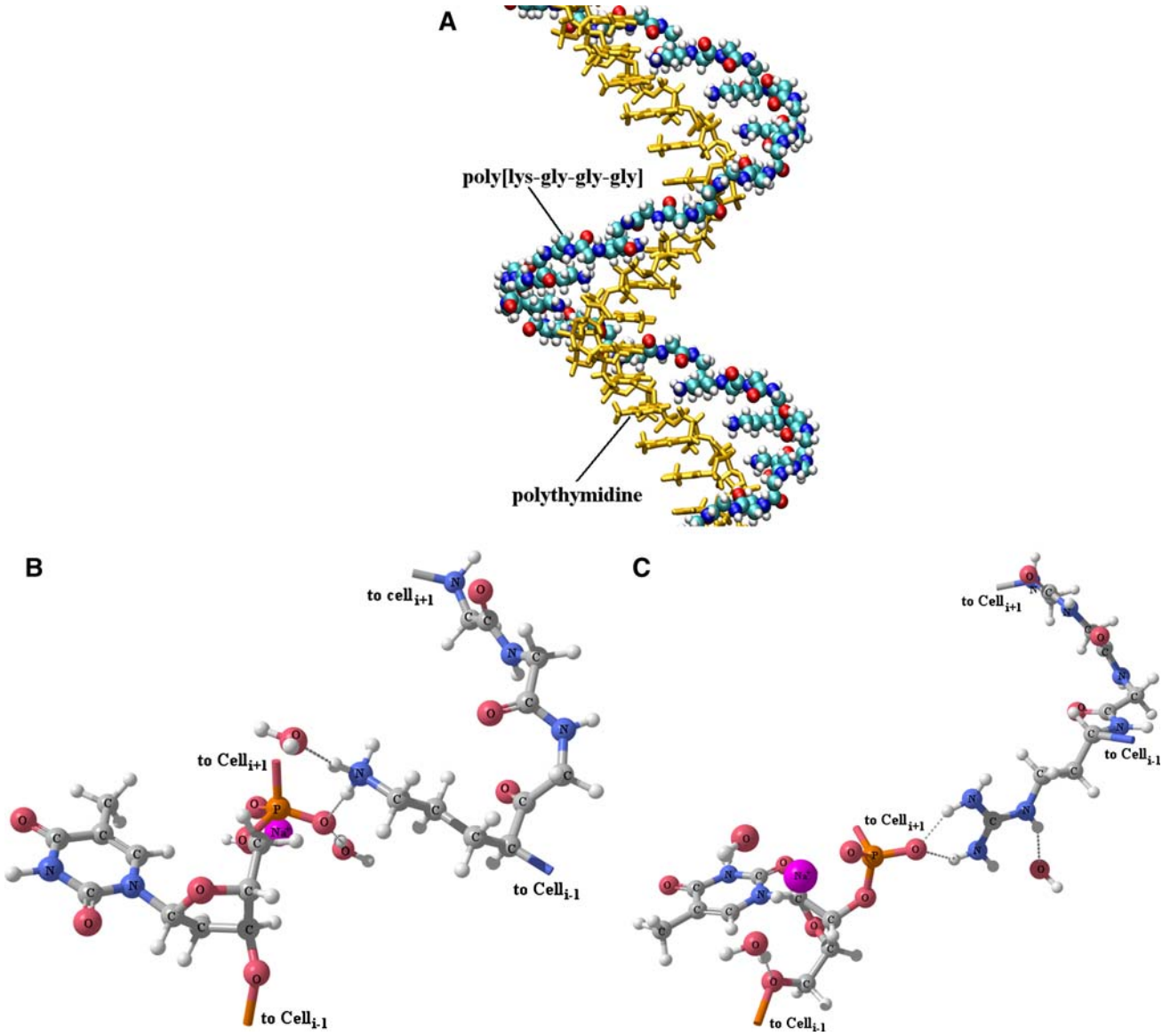

Fig. 1 **a** The spatial structure of the polythymidine-poly[*lys-gly-gly-gly*] model system (sticks: polythymidine, balls: poly[*lys-gly-gly-gly*]), **b** the unit cell of the model system with *lys*, **c** the unit cell of the model system with *arg*. H-bonds between the nucleotide and the charged amino acids are indicated by *dotted lines*

features of this complicated biomolecular complex. In our model the protein is substituted with a periodic polypeptide consisting of X-*gly*-*gly*-*gly* repeat units (X is either *lys* or *arg*). This chain follows the single-stranded homopolynucleotide built of thymidine (Fig. 1a). The repeat units of these two model systems are presented in Fig. 1b and c. Although our model is geometrically different from the nucleosome structure, it has two important features. On the one hand, every PO_4^- group is H-bonded by a positively charged amino acid residue (lys^+ or arg^+) (in fact our model overestimates the number of these H-bonds). On the other hand, the application of the periodic boundary condition makes it possible to consider large (in fact infinite) number of these interactions, and allows us to decide whether solid-state physical effects are as important in the CT of this system as they are in the previously mentioned TCNQ–TTF case.

For the infinite chain calculations we have applied the ab initio HF crystal orbital (CO) method in its general form applicable to any one-dimensional (1D) system [12]. The COs were determined in the linear combination of atomic orbitals (LCAO) approximation as it is implemented in an extended version of J. Mintmire's PolyXα code [29]. For further details see [11, 30].

The unit cells of the infinite chains were built in the following manner: the geometry of thymine, sugar-phosphate group, *lys* (or *arg*), water and Na^+ (Clementi's basis set for the K atom was not available. Therefore we changed the K^+ ion to Na^+) ions were taken as is described in [17] and additionally three *gly* molecules were used to connect the single *lys* (or *arg*). The three-*gly* bridge was optimized using the Gaussian 03 program package [31]. During this procedure, we have considered only the *lys* (or *arg*) and triglycine part of three subsequent unit cells, and kept the atoms of the *lys* (or *arg*) molecules frozen.

In our earlier studies [16, 17] the TZVP basis set was used, which is too large for the infinite chain calculation for our model systems. We had to choose smaller basis sets, which were Clementi's double ξ (CDZ) [25] and the simple 6-31G basis sets [32–34]. To the former one we also added either a set of diffuse 2*p* or a set of diffuse *d* functions on the heavy atoms of T. Since these basis functions spread out more into the space between the stacked molecules, they increase the overlap of the π orbitals of the stacked T molecules. Therefore we expected that this would better describe the CT between the DNA–histones systems. To test the capability of these smaller basis sets to describe the CT in our systems, we calculated the CT values of thymidine–*lys*/*arg* complex with them and compared the results to those obtained earlier with the TZVP basis set.

The Mulliken populations (and with it the CTs) for a single unit of thymidine and the *lys* or *arg* containing parts of the model chain have not changed. Therefore we have introduced also a non-standard basis set tailored for stacked systems. Instead of changing the basis set for the T atoms in polythymidine, we have introduced a "phantom" T molecule half way between the two T molecules (1.66 Å) and at a rotational angle of 18°. On the nuclei of these phantom T molecules (which do not exist at all, rather only provide additional basis functions for a better description) we have centered a set of additional *p* functions [35].

As we shall see, even with the help of most of these basis set modifications, the transferred charge remains nearly the same (see "Results and discussion"). Only the phantom basis set increases the CT. The reason for this is that to keep charge neutrality in the infinite chains, in contrast to the monomer, where we had three H_2O molecules and one K^+ ion between the chains, we had to put two H_2O molecules, one $O\bar{H}$ ion and a Na^+ ion between them in every unit cell.

Finally, it should be mentioned that we could use neither the counterpoise method to correct the basis set superposition errors (BSSE), nor the natural bond orbital (NBO) method for population analysis [23, 24] in the case of the infinite chains, because neither of these two methods is compatible with the available band structure program for one-dimensional chains.

3 Results and discussion

In Table 1 we present the results of CT calculations using Clementi's double ξ [25] and 6–31G basis sets. Additionally, for the sake of comparison, our previous results obtained with the TZVP basis [21] for the thymidine–*lys* or *arg* pairs are also listed. The HF–Mulliken CT values calculated in the CDZ basis set are somewhat larger than

Table 1 The charge transfer from PO_4^- to lysine$^+$ or arginine$^+$ in the thymidine-lysine (arginine) complex calculated with different methods and basis sets

	HF		MP2	
	Mulliken	NBO	Mulliken	NBO
Lysine				
Clementi's doule ξ	0.16	0.10	–	–
6–31G	0.10	0.09	–	–
TZVP[a] with screening	0.07	0.05	0.10	0.07
TZVP[a] without screening	0.14	–	0.26	–
Arginine				
Clementi's doule ξ	0.16	0.10	–	–
6–31G	0.12	0.10	–	–
TZVP[a] with screening	0.08	0.04	0.08	0.05
TZVP [21][a] without screening	0.15	–	0.21	–

[a] See Refs. [10, 11]

Table 2 The valence band upper edges, the conduction band lower edges, the gaps (all in eV) and the charge transfer from the PO_4^- groups of polythymidine to the lysine$^+$ or arginine$^+$ side chains of the poly(lysine/arginine–triglycine) system with different basis sets (in *e* units)

	Valence band upper edge	Conduction band lower edge	Gap	Charge transfer
Lysine				
Basis set				
Clementi's double ξ	−9.78	0.92	10.70	0.16
6-31G	−7.37	2.42	9.79	0.10
Clementi's double ξ + extra set of diffuse *p* functions (orb. Exp. 0.1)	−8.99	1.96	10.95	0.15
Clementi's double ξ + extra set of diffuse *d* functions (orb. Exp. 0.1)	−8.96	1.96	10.92	0.15
Clementi's double ξ + "phantom" molecule	−8.96	1.95	10.91	0.15
Arginine				
Basis set				
Clementi's double ξ	−7.74	2.53	10.27	0.12
6-31G	−7.37	2.42	9.79	0.10
Clementi's double ξ + extra set of diffuse *p* functions (orb. Exp. 0.1)	−6.92	3.39	10.31	0.12
Clementi's double ξ + extra set of diffuse *d* functions (orb. Exp. 0.1)	−6.95	3.39	10.34	0.12
Clementi's double ξ + "phantom" molecule	−6.93	3.39	10.32	0.12

those obtained with 6–31G basis set, while the NBO CT values are almost the same for both basis sets. The Mulliken CT is larger in every investigated case. One can also observe that with screening the CT decreases by a factor of about two if one uses a better basis (like TZVP) in the HF case both for *lys* and *arg*. In the case of MP2 the effect is even stronger (CT decreases by a factor of 2.5 for both *lys* and *arg*).

In Table 2 we present the main characteristics (valence band upper edge, conduction band lower edge, gap and CT) of the band structures of the polythymidine–poly[lysine (or arginine)–triglycine] system and the charge transfers between them. For our calculations we have used the crystal orbital method in its LCAO form (see "Methods").

The CT values calculated using the CDZ basis set are somewhat larger (0.16 and 0.12 *e* for *lys* and *arg*, respectively) than those with the 6–31G basis sets (0.10 *e* for both *lys* and *arg*). Neither the addition of diffuse *p* and *d* functions to the CDZ basis set nor the usage of the phantom atoms changed the CT values significantly. One should mention that a small fraction of the Mulliken populations of the other atoms (0.01–0.02 *e*) appear on them. We have added these charges to the total charge of thymidine. We find that for most basis sets the CT increases as compared to its unscreened HF values (see the TZVP rows of Table 1). Most probably the main reasons behind this are not different solid-state physical effects, but the presence of the Na^+ and $O\bar{H}$ ions that could be added for obvious reasons (an infinite chain must be calculated with neutral unit cells). With these $O\bar{H}$ ions the interactions between the units of polythymidine and poly[lysine (or arginine)-triglycine] became unscreened.

Turning to the band structures in the case of the composite chain (see Table 2) we have chosen as valence band the highest filled energy band with a width larger than 10×0.026 eV $= 0.26$ eV to be able to use the deformation potential approximation for the calculation of its transport [36–38]. We selected the conduction band on the basis of the same criterion. Between these bands there are three or four extremely narrow bands which do not contain contributions from the basis functions of thymine. Because of their narrowness they cannot play any role in Bloch-type conduction in these systems.

From Table 2 one finds an average charge transfer of 0.13 *e* in the case of *lys* and 0.12 *e* in the case of *arg*, respectively, based on Mulliken population analysis. The average NBO CT values for *lys* are $0.13 \times 0.77\ e = 0.086\ e$ and in the case of *arg* $0.12 \times 0.67\ e = 0.080\ e$ (for the used

Table 3 The position and width of the conduction and valence bands of poly[lysine–triglycine] and poly[arginine–triglycine] systems together with their band gaps (in eV)

	Valence band upper edge	Width	Conduction band lower edge	Width	Gap
poly[*lys-gly-gly-gly*]	−11.69	0.10	−0.18	0.29	11.51
poly[*arg-gly-gly-gly*]	−11.17	0.09	2.52	0.05	13.69

NBO values see Table 1). These values have to be multiplied by $\frac{120}{147}$ (120 sites in the 147 base pairs long DNA superhelix in a nucleosome which forms H bonds with the nucleohistones [4]) and by 0.5 because our calculation refers to a DNA single helix $\left\{ \begin{matrix} 0.10e \\ 0.08e \end{matrix} \right\} \times \frac{120}{147} \times 0.5 = \left\{ \begin{matrix} 0.04e \\ 0.03e \end{matrix} \right\}$ CT/nucleotide base (the first value refers to *lys*, the second one to *arg*). This value is rather small, but one should not forget that it occurs at a large number of places even within a single nucleosome. Furthermore, since the infinite chain calculations did not include electron correlation, one should expect an increase of CT for the unit cell about 20%, which would change the CT to $0.10e - 0.15e$ if one uses the MP2 method. Since, however, we have no electron correlation data in the case of the infinite chains, we prefer not to attempt to increase the CT on this basis.

In the cases of *lys* or *arg*, respectively, we have constructed two model chains: poly[lysine–triglycine] and poly[arginine–triglycine]. As mentioned earlier, these model chains have the same curvature as polythymidine (see Fig. 1a). We have performed band structure calculations also for these two model protein chains (see Table 3).

In the case of the model protein chains only the one with *lys* has a conduction band broad enough (0.29 eV) for Bloch-type conduction.

The distance between the upper edge of the valence band of the composite system and the lower edge of the conduction band of the *lys* containing model polypeptide chain is still 6.74 eV even if we add an extra set of *p* functions to the heavy atoms of thymine with the small orbital exponent of 0.1. This is far too large to suppose a CT between these two chains even if one used a better basis set and introduces electron correlation.

4 Conclusions

One can conclude that between an infinite homopolynucleotide chain and an infinite periodic protein chain no direct charge transfer can occur even if the components are charged (like the PO_4^- group on the DNA side and the lys^+ or arg^+ groups of a protein chain). The reason for this is that the distance between the valence band of the homopolynucleotide and the model peptide chain is too large (6.7 eV). The resulting small CT is obviously caused by charge rearrangement of the composite system.

The solution to this problem is that in reality neither a polynucleotide chain, nor a polypeptide chain is periodic. It is well known that in multicomponent aperiodic systems (because of the many different kinds of interactions between the neighboring units) the electronic density of states profile (DOS) can broaden very much which has been demonstrated in the case of DNA [39]. In this way, the strongly broadened bands of both aperiodic chains can easily overlap. The charge transfer can occur and a hopping conduction can take place if strong enough local electric fields are present in the neighborhood of the two interacting chains. For this reason, we intend to perform CT calculations between two aperiodic chains *utilizing* a proper hopping mechanism [40].

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