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Molecular Dynamics Simulations of The DNA Radiation Damage and Conformation Behavior on A Zirconium Dioxide Surface

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THIS work is aimed on a complex study of the DNA immobilization and conformation processes on the zirconium dioxide (ZrO_2) surface. The DNA+ZrO_2 nanoparticles and nanosized films were investigated with the molecular dynamics (MD) modeling, experimental spectral and integral methods, including nuclear physics. Using the MD hybrid classical and quantum chemistry potentials, for the DNA solvated with water the DNA+ZrO_2 surface interactions were simulated We have generated series MD models, thereby simulating a different scenario of the DNA with possible charge modifications. The DNA charge modification were introduced in the DNA central region via its two phosphorus atoms, P_a and P_b, and for several set of MD models for the relaxed DNA structures we have estimated the positional changes of the distance D[DNA(P_a,P_b) - ZrO_2(O)] between the phosphorus atoms (P_a,P_b) and selected oxygen atoms of the ZrO_2 surface. The work is aimed to the development of functional heterojunctions such as a biological molecule - wide-gap dielectric. These heterojunctions are intended for useing in the field of molecular electronics, in particular, for the creation of biochips, memory arrays and computer architectures of the future.

Keywords: DNA radiation; DNA conformation and immobilization on the surface, zirconium dioxide; modular dynamics modeling.

Introduction

Molecular modeling including molecualr dynamics and/or electronic structure methods [1-2] is widely applied to investigate many systesm not limited to chemistry, physics, biology and envrioenmt. Emerging materials as well as biological molecules are considered among the most important molecular systems achived by molecualr modeling [3-8]. The combination of biomolecules with solid nanoparticles generates a new class of materials, primarily for new electronic sensory and optical systems, the prospects for the development of molecular electronics, the creation of biochips, memory arrays and computer architectures of the future become real. DNA molecules have good electrical conductivity, are able to store and transmit by copying terabytes of information self-reproducing and moving in the electric field, therefore, are extremely interesting as a functional element of bioelectronic devices [9-16]. Zirconium dioxide is a promising material as a DNA molecules adsorber due to good biocompatibility and high dielectric constant (ε=25). Wherein, the questions of interaction with this material of DNA molecules have not

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been studied yet [9-16]. The purpose of this work is to obtain biologically modified structures by immobilizing of DNA molecules on the surface of biocompatible crystals, an experimental and theoretical study of the fundamental mechanisms of physico-chemical interaction and dynamics of the DNA molecule on interfaces with solid bases under the influence of external electric fields and radiation fluxes. Based upon the above consideratiosn as well as previous findings [17-20], the presnt work is onducted. The tasks of this work are to include simulations of radiation induced conformations for the DNA chian on a zirconia dioxide surface by MD (molecular dynamics) method.

MD simulation details and struture building

For a triple system DNA + water + ZrO_2 surface, all the interatomic interactions are described with standard molecular mechanics potentials, as a sum of two-, three-, and four atom terms. All-atom interactions include harmonic bonds, angles, improper torsions, and dihedral angles. The long-range interactions include Lennard-Jones van der Waals potentials and electrostatic potentials between atom-based partial charges [21-22]:

$$U(r) = U_b + U_\theta + U_\varphi + U_\omega + U_{LJ} + U_{el} + U_{HB} + \dots ,$$

Here valence length potential, $U_b = \frac{1}{2}\sum_b K_b\,(r - b_0)^2$, the valence angle potential, $U_\theta = \frac{1}{2}\sum_\theta K_\theta\,(\theta - \theta_0)^2$, the torsion dihedral potential, $U_\varphi = \frac{1}{2}\sum_\varphi K_\varphi[\cos(n\varphi - \delta) + 1]$, the Van-der-Waals interaction and hydrogen bonding potentials are Lennard-Jones (LJ; 12-6) or (12-10) types, $U_{LJ} = \sum_{i,j}\left[\frac{A}{r_{ij}^{12}} - \frac{B}{r_{ij}^{6}}\right]$ and $U_{HB} = \sum_{i,j}\left[\frac{A'}{r_{ij}^{12}} - \frac{B'}{r_{ij}^{10}}\right]$, the electrostatics potential, $U_{el} = \sum_{i,j}\frac{q_i q_j}{\varepsilon r_{ij}}$, represents long-range interactions in the system. For the DNA solvated with water, based on the experimental data, *ab initio* and semiempirical electronic structure calculations, a number of self-consistent and well-tested sets of parameters are published and available (see, for example, all-atom sets in CHARMm22; Brooks et al., 1983). For ZrO_2 surface we have used Buckingham interaction potential, $U(r) = A\exp\left(-\frac{r}{\rho}\right) - \frac{C}{r^6}$ with the interaction parameters *A, C* and ρ [23-24].

All the potential parameters used in the MD simulations are listed in our previous papers (Refs. [25-26]). In Fig. 1(a,b) the initial position of a DNA chain on ZrO_2 (zirconia dioxide) surface and the whole system solvated with water are shown, respectively.

The DNA chain was located at a well-separated distance from the zirconia dioxide. After appropriate preparation of the DNA+ZrO_2 surface a water box was introduced. The DNA+ZrO_2 system was solvated with a SPC water box and relaxed for 500 ps at fixed a DNA position upon ZrO_2 surface. The MD relaxation process was reproduced by an isothermal NVT ensemble, in which the number of particles, volume, and temperature are fixed. The total system DNA+ZrO_2+water temperature was controlled with the NVT the Nosé-Hoover thermostat at T=310 K with a relaxation time of 1.0 ps. A 9 Å cutoff is used for non-bonded forces together with the particle mesh Ewald method for calculating of the long-range electrostatic interactions. A rectangular box of dimensions 60.0 Å by 90.0 Å by 64.5 Å which contained a single DNA molecule (1260 chemically bonded P, C, N, O, H atoms), 1152 zirconia dioxide surface molecules (384 zirconium and 768 oxygen atoms) and 3200 water molecules (3200x3=9600 OW and HW atoms) was subjected at the equilibration steps as described above under multiple MD run. For all the conducted simulations a time step of 1 fs was used for the integration of the equation of motion with Verlet leapfrog integrator. The covalent bonds involving hydrogen atoms constrained using SHAKE algorithm. The MD trajectory calculations performed for multiple DNA+water+ZrO_2 models were next used to simulate the effect of the radiation introduced on a DNA side chain with consequent conformation changes [25-26].

For the DNA molecule solvated with water and interacting with the ZrO_2 surface we have consider different model structures, thereby simulating different scenario of the DNA possible charge modification. From two opposite DNA directions we have arbitrarily chosen two P (phosphorus) atoms as shown in Fig. 2-3 as possible damage sites. The DNA charge modification we have

introduced in its central region through two set of MD models (set A and B) for both phosphorus atoms P_a and P_b as follows: **set A** (Model 1 (native DNA): $Q(P_a) = +1{,}1659|e|$; Model 2 (damaged DNA): $Q(P_a) = 0$; Model 3 (damaged DNA): $Q(P_a) = -1{,}1659|e|$), **set B** (Model 4 (native DNA): $Q(P_b) = +1{,}1659|e|$; Model 5 (damaged DNA): $Q(P_b) = 0$; Model 6 (damaged DNA): $Q(P_b) = -1{,}1659|e|$), where e is electron charge.

The above choice of phosphates in the DNA charge modification introduced were due to the DNA-ZrO_2 surface interactions as in paper: J.Phys. Chem. B, 2015, 119 (11030-11040),(https://pubs.acs.org/doi/10.1021/acs.jpcb.5b01983); where the authors have studied via molecular dynamics simulations several DNA phosphate and surface silanol groups, hydrophobic bonding between DNA base and silica hydrophobic region. Also, they have found two major binding mechanisms to be attractive interactions between DNA phosphate and surface silanol groups, hydrophobic bonding between DNA base and

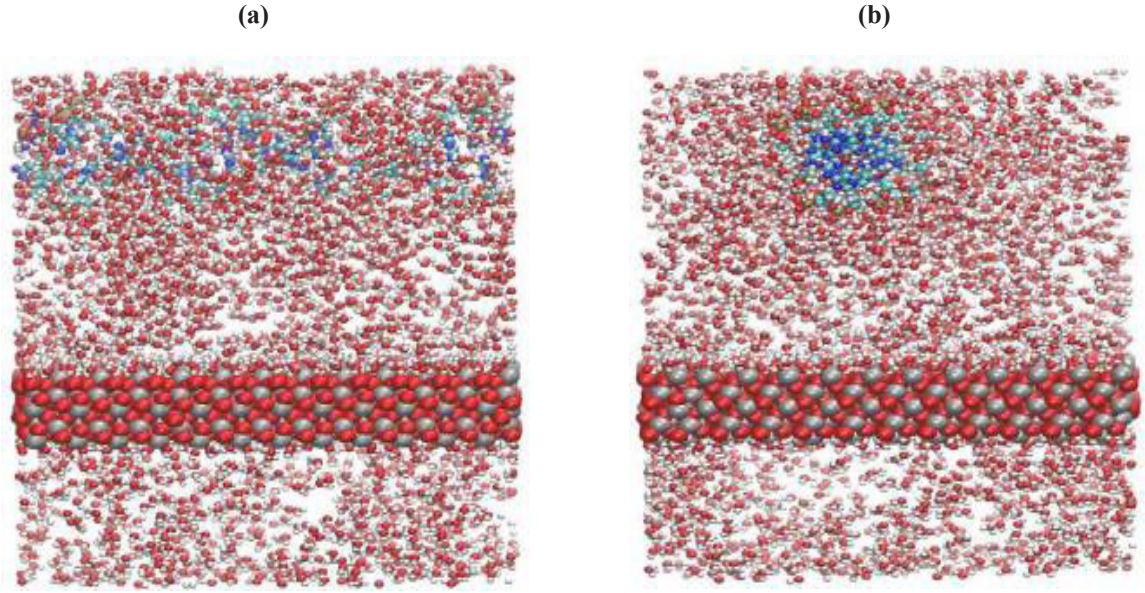

Fig. 1(a, b). The system (DNA molecule and ZrO_2 surface) solvated with water.

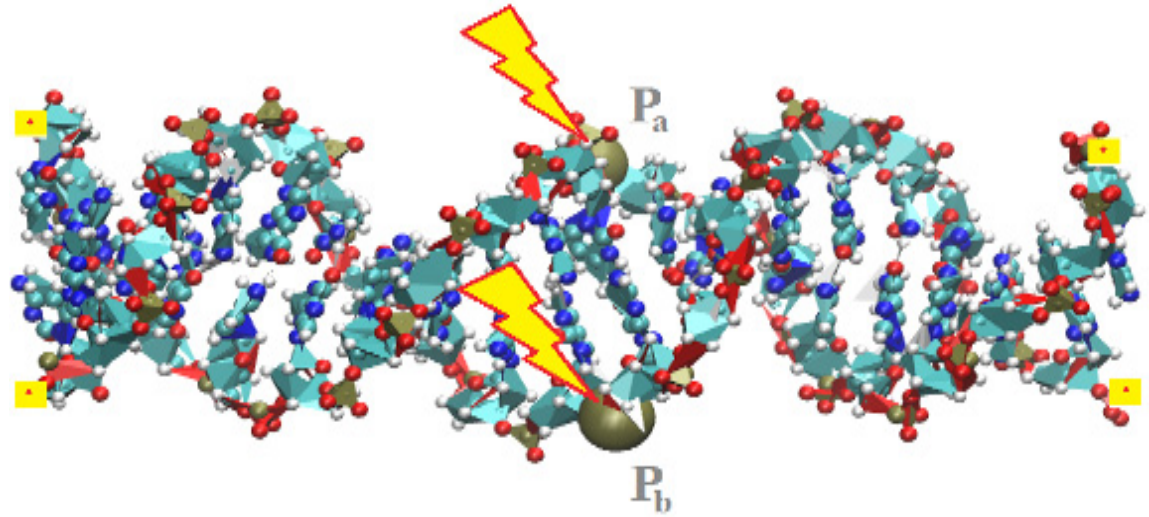

Fig. 2. The position of two P (phosphorus) atoms (P_a and P_b; grey color) of the DNA molecule are shown as possibly DNA damaged sites.

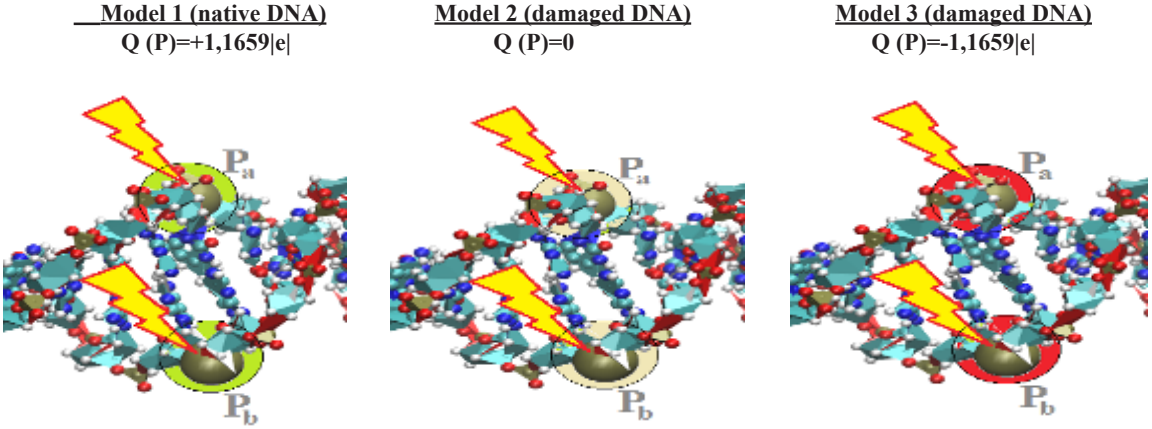

Fig. 3. The charge modification on two P (phosphorus) atoms of the DNA damaged sites.

silica hydrophobic region (Fig. 2-3).

The MD simulation results

A general view of the DNA and ZrO_2 surface is shown in Fig. 4(a,b), where in the water solvated system the position of two phosphorus atoms (grey color) of DNA molecule and one oxygen atom (red color) of ZrO_2 surface are indentified.

It should be noted that for all above set of MD models with the DNA relaxation procedure we have estimate the positional changes of the distance D[DNA(P_a, P_b) - ZrO_2(O)] between the phosphorus atoms (P_a, P_b) and selected oxygen atoms of the ZrO_2 surface (Fig. 6(a,b)). In Fig. 5 the MD simulation results for the D[DNA(P_a) - ZrO_2(O)] dynamics are shown for the models 1-3. The distance distribution D[DNA(P_a) - ZrO_2(O)] between the phosphorus (P_a) and selected oxygen (O) atoms of the zirconium dioxide surface are compared for the native DNA (model 1: Q(P_a)=+1,1659|e|) and two damaged versions (models 2: Q(P_a)=0 and 3: Q(P_a)=-1,1659|e|). The charge state of the phosphorus (P_a, P_b) atoms mimics the effect of external radiation (UV or other) induced on the site of DNA, such that the value of Q(P_a) spontaneously vary in the interval [+1,1659;-1,1659]|e|. From the distance diagrams in Fig. 5 we can see both different D[DNA(P_a) - ZrO_2(O)] time dependent behavior and different DNA-surface close contact on a final state.

So far, starting from the same relaxed state (but with different Q(P_a)) the DNA molecule while interacting with ZrO_2 surface will undergo a different conformational shape, thereby approaching the surface. Below Fig.s 6-8 compare the DNA conformational behavior (top: side view, middle: up view; bottom: on the surface) at the initial and final states. The DNA orientation dynamics on ZrO_2 in Fig.6-8 are presented for the model 1 (native DNA): Q(P_a) = +1,1659|e| and two damaged versions (models 2: Q(P_a)=0 and 3: Q(P_a)=-1,1659|e|), respectively.

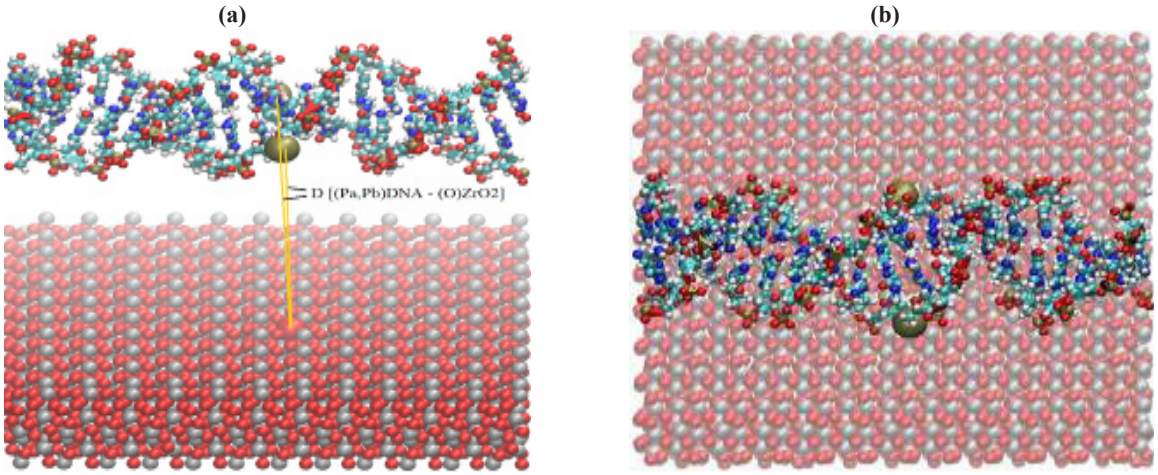

Fig. 4 (a, b). The position of two phosphorus atoms of DNA molecule and one oxygen atom of ZrO_2 surface are shown.

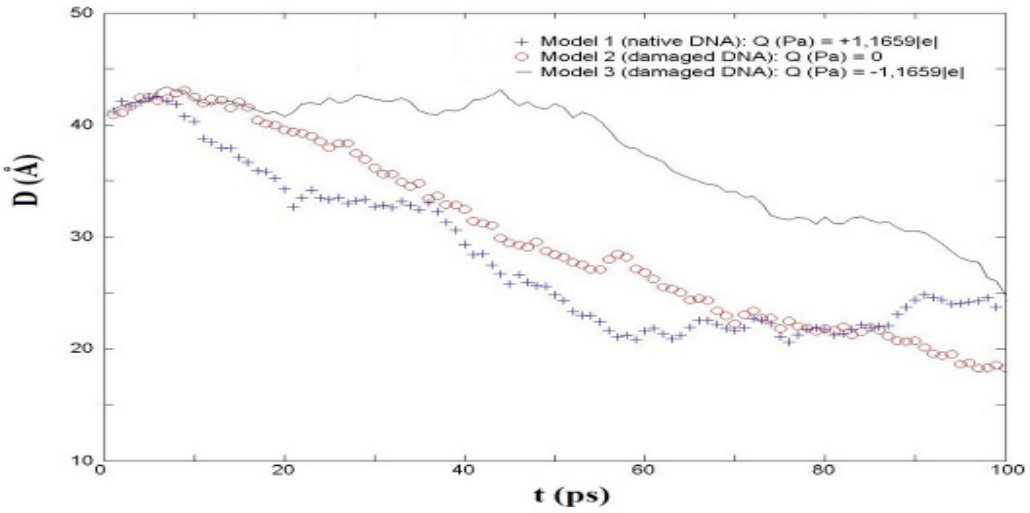

Fig. 5. The distance D[DNA(P_a) - ZrO_2(O)] between phosphorus (P_a) and selected oxygen (O) atoms of the zirconium dioxide surface for the MD models 1-2-3.

Model 1 (native DNA): Q(P_a)=+1,1659|e|

t=0 **t=100 ps**

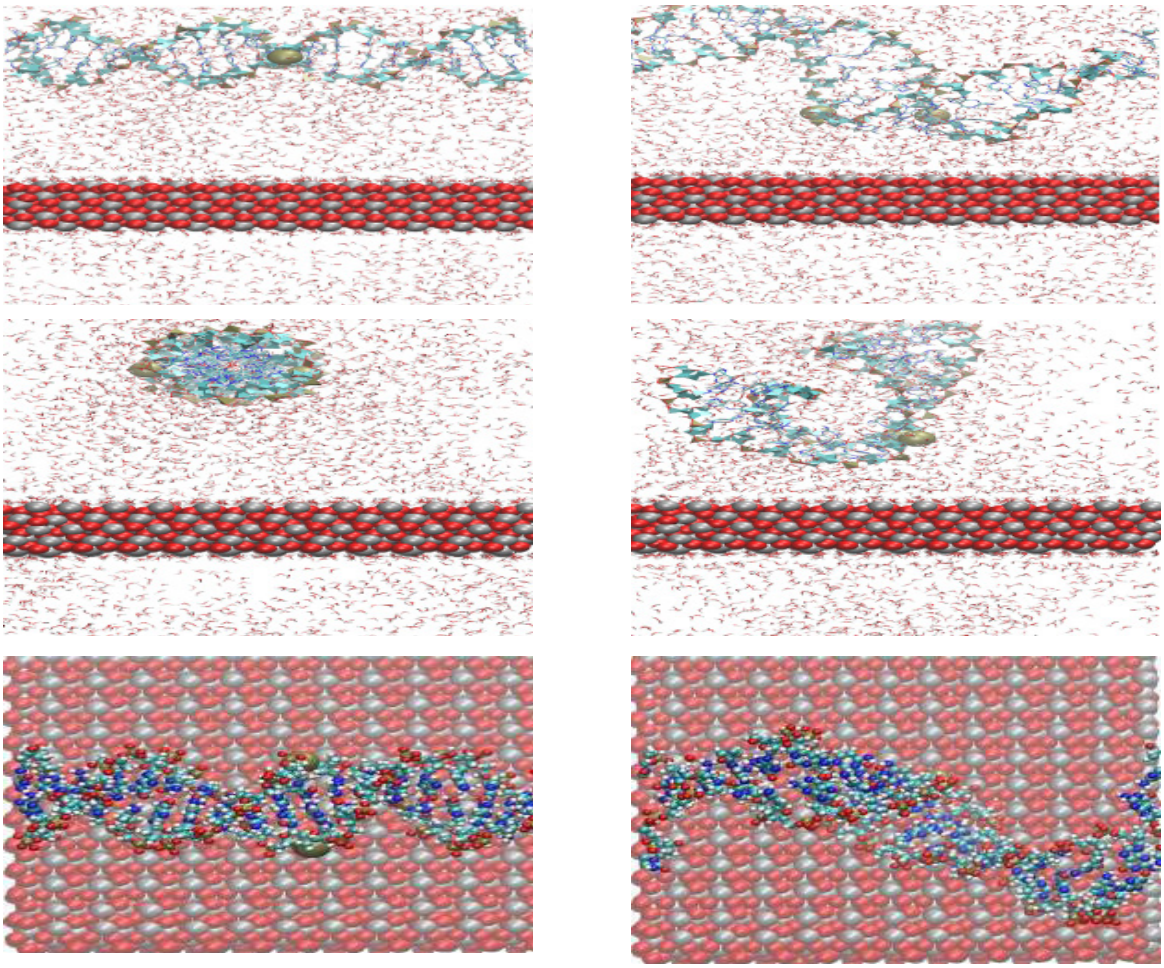

Fig. 6. The DNA orientation dynamics on ZrO_2 for model 1 (native DNA): Q(P_a)=+1,1659|e|

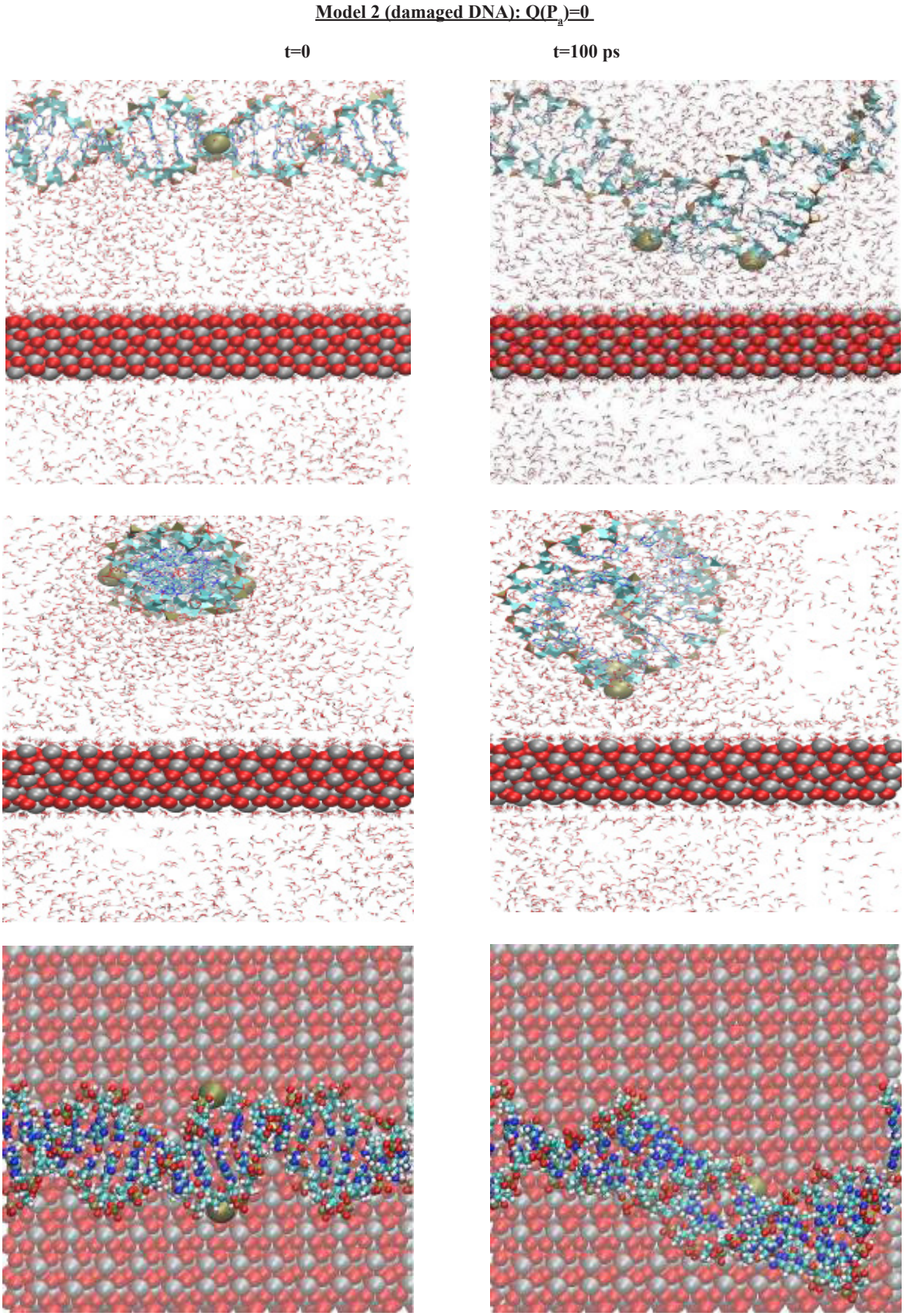

Fig. 7. The DNA orientation dynamics on ZrO_2 for model 3 (damaged DNA): Q(P_a)=0.

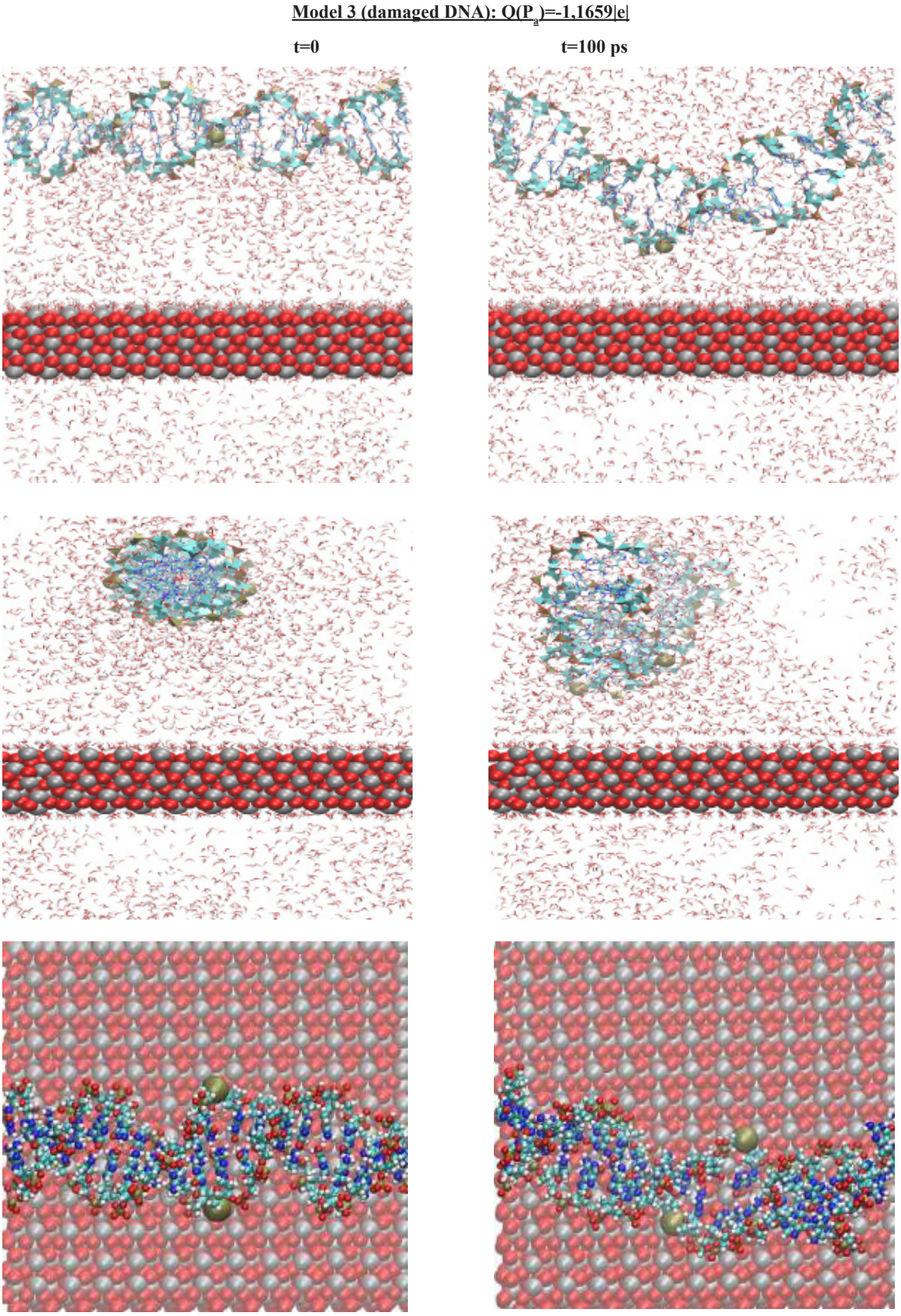

Fig. 8. The DNA orientation dynamics on ZrO_2 for model 2 (damaged DNA): Q(P_a)=-1,1659|e|.

In Fig. 9 the MD simulation results for the D[DNA(P_b) - ZrO_2(O)] dynamics are shown for the models 4-6. The distance distribution D[DNA(P_b) - ZrO_2(O)] between the phosphorus (P_b) and selected oxygen (O) atoms of the zirconium dioxide surface are compared for the native DNA (model 4: Q(P_b)=+1,1659|e|) and two damaged versions (models 5: Q(P_b)=0 and 6: Q(P_b)=-1,1659|e|).

Below Fig. 10-11 compare the DNA conformational behavior (top: side view, middle: up view; bottom: on the surface) at the initial and final states. The DNA orientation dynamics on ZrO_2 in Fig.10-11 are presented for two damaged DNA models 5: Q(P_b)=0 and 6: Q(P_b)=-1,1659|e|), respectively For the model 4 (native DNA; Q(P_b)=+1,1659|e|) the results are similar as shown in Fig. 6 above. The MD results compare the DNA conformational behavior at the initial and final states and the DNA orientation dynamics on ZrO_2 were presented for the native DNA (Q(P_a, P_b) = +1,1659|e|) and two damaged versions (Q(P_a, P_b)=0 and Q(P_a, P_b)=-1,1659|e|), respectively. So far, starting from the same relaxed state (but with different Q(Pa,Pb) the DNA molecule while interacting with ZrO_2 surface will undergo a different conformational shape, thereby approaching the surface. We have related the DNA molecular orientations due to the immobilization process or similar to the DNA B-Z-transition happening on the zirconium dioxide (ZrO_2) surface. The DNA conformations arise when the relative orientation of individual parts of the molecule changes as a result of the rotation of atoms or groups of atoms around simple bonds, bending of bonds, etc. For example, the DNA B-Z-transition can be stimulated by an increase in the content of ions in solution (say, zirconium dioxide ZrO_2 surface) or by certain proteins that stabilize the Z-form of DNA. When a molecule transitions from B- to Z-form, the double helix of DNA unfolds, and then turns in the other direction, turning from right-wound into left-wound [27-28].

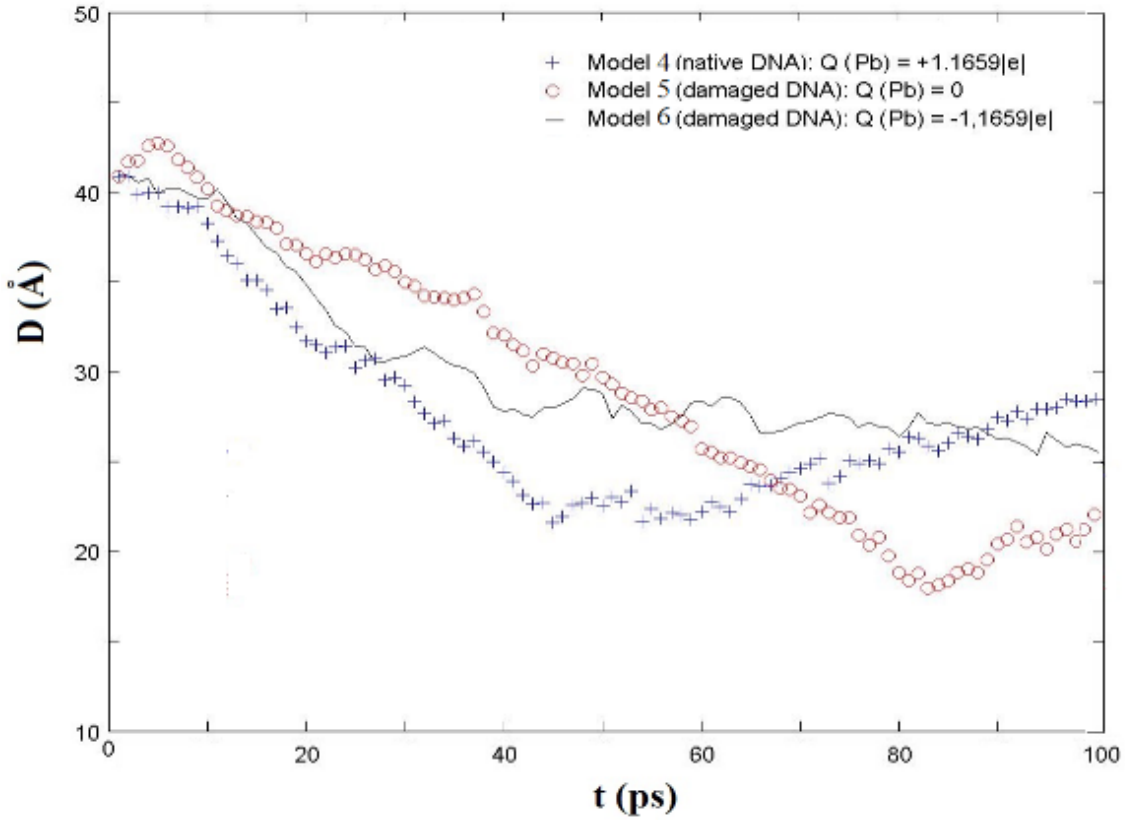

Fig. 9. The distance D[DNA(P_b) - ZrO_2(O)] between phosphorus (P_b) and selected oxygen (O) atoms of the zirconium dioxide surface for the MD models 4-5-6.

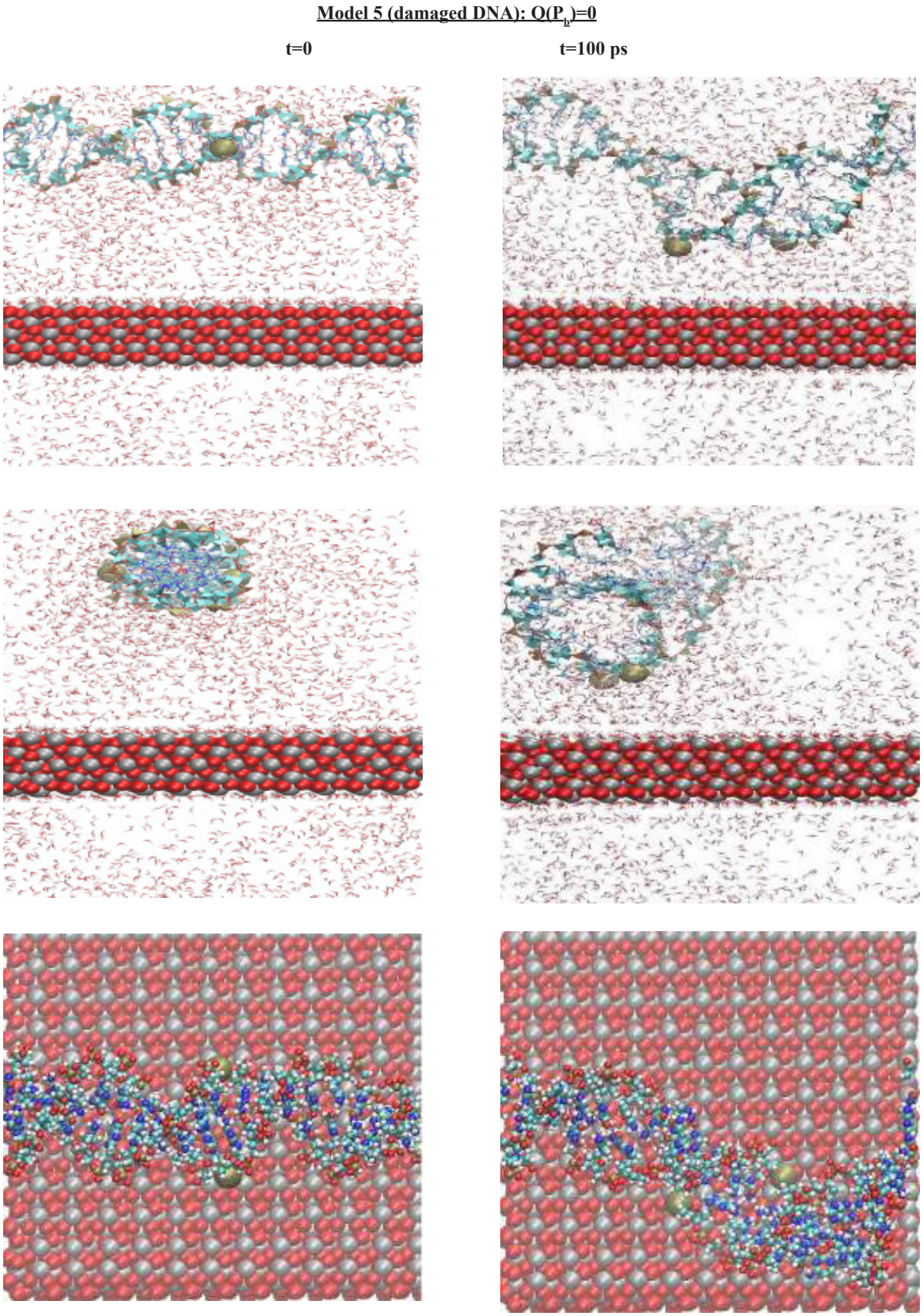

Fig. 10. The DNA orientation dynamics on ZrO_2 for model 6 (damaged DNA): $Q(P_b)=0$.

Model 6 (damaged DNA): Q(P_b)=-1,1659|e|

t=0 **t=100 ps**

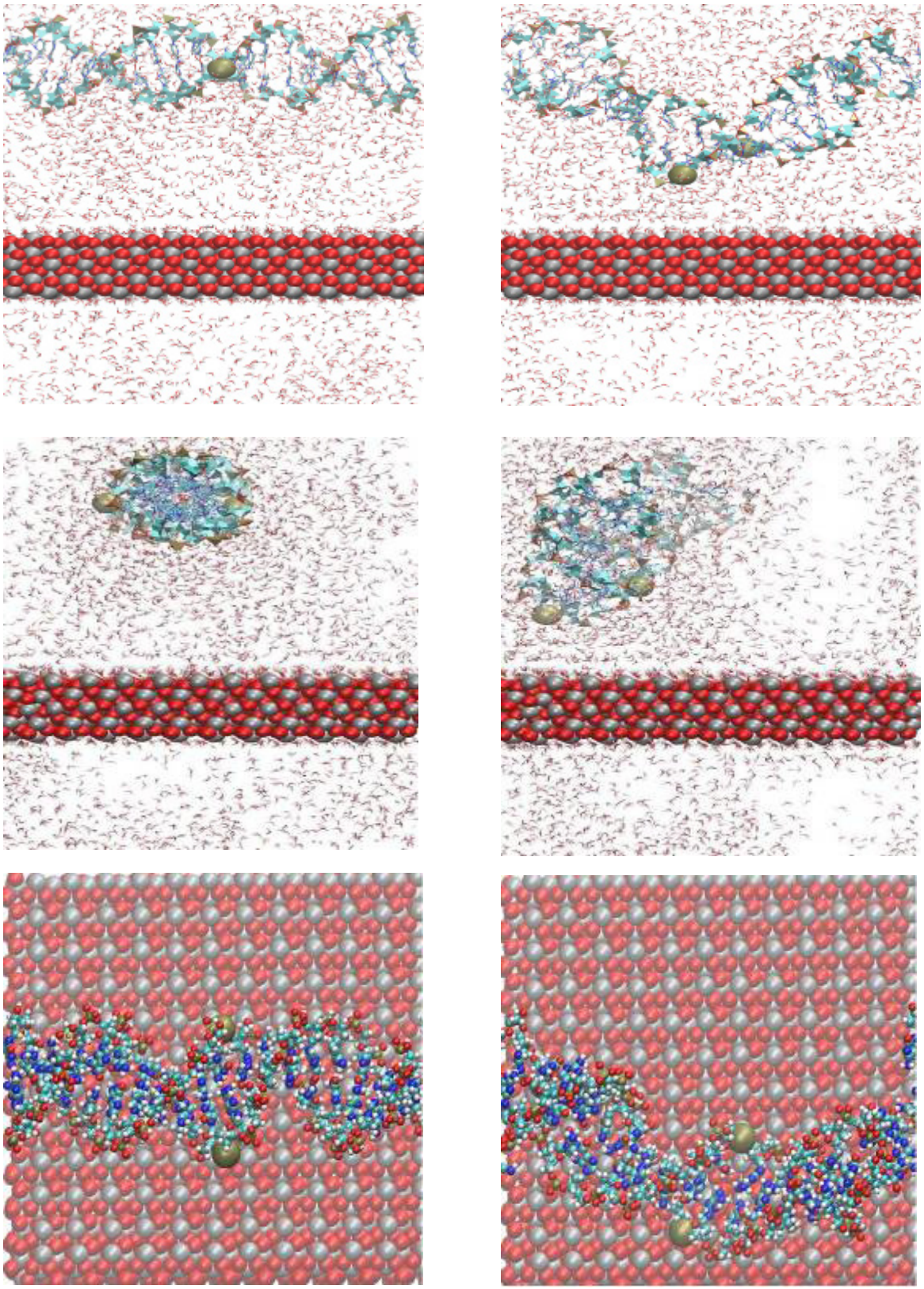

Fig. 11. The DNA orientation dynamics on ZrO_2 for model 5 (damaged DNA): Q(P_b)=-1,1659|e|.

Conclusion

For a triple system DNA + water + ZrO_2 surface we built several set of MD models as **set A** (Model 1 (native DNA): $Q(P_a)$=+1,1659|e|; Model 2 (damaged DNA): $Q(P_a)$=0; Model 3 (damaged DNA): $Q(P_a)$=-1,1659|e|) and **set B** (Model 4 (native DNA): $Q(P_b)$=+1,1659|e|; Model 5 (damaged DNA): $Q(P_b)$=0; Model 6 (damaged DNA): $Q(P_b)$=-1,1659|e|), where e is electron charge), thereby simulating different scenario of the DNA possible charge modification. From two opposite DNA directions we have arbitrarily chosen two P (phosphorus) atoms as possible damage sites. The MD results compare the DNA conformational behavior at the initial and final states and the DNA orientation dynamics on ZrO_2 were presented for the native DNA ($Q(P_a,P_b)$ = +1,1659|e|) and two damaged versions ($Q(P_a,P_b)$=0 and $Q(P_a,P_b)$=-1,1659|e|), respectively. So far, starting from the same relaxed state (but with different $Q(P_a,P_b)$ the DNA molecule while interacting with ZrO_2 surface will undergo a different conformational shape, thereby approaching the surface.

In conclusion, for today the DNA+ZrO_2 system emerges itself as a breakthrough potential material for developing new nano-bio-electronics tools as well as the interdisciplinary research target in the field of nanotechnology. Wherein, the questions of the DNA interaction and immobilization with the mentioned oxide material as ZrO_2 have not been studied yet. The obtained results for the DNA conformational behavior through the MD simulation analysis provide a novel picture for the DNA/ZrO_2 interaction and immobilization processes at the atomic/molecular level. The zirconium dioxide (ZrO_2) has seen to be a promising material as DNA or RNA molecules absorber due to a good biocompatibility and a high dielectric constant (å=25). For today the combination of bio-molecules with solid nano-particles generates a new class of materials, primarily for new electronic sensory and optical systems. The prospects cover the development of molecular electronics, the creation of biochips, memory arrays and future computer architectures as well. In this respect, the DNA and RNA molecules have good electrical conductivity, capable to store and transmit by copying terabytes of information with self-reproducing and moving in the electric field, therefore, are extremely interesting as a functional element of bio-electronic devices [23-24].

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References

1. Hosseini-Hashemi S., Sepahi-Boroujeni A., Sepahi-Boroujeni. S.; Analytical and molecular dynamics studies on the impact loading of single-layered graphene sheet by fullerene, *Appl. Surf. Sci.*, **437**, 366-374 (2018).

2. Belghiti M.E., Echihi S., Mahsoune A., Karzazi Y., Aboulmouhajir A., Dafali A., Bahadur I.; Piperine derivatives as green corrosion inhibitors on iron surface; DFT, Monte Carlo dynamics study and complexation modes, *J. Mol. Liq.*, **261**, 62-75 (2018).

3. Ibrahim M., Osman, O; Spectroscopic analyses of cellulose: Fourier transform infrared and molecular modelling study, *J. Comput. Theor. Nanosci.*, **6**(5), 1054-1058 (2009).

4. Ibrahim M.; Molecular modeling and FTIR study for K, Na, Ca and Mg coordination with organic acid, *J. Comput. Theor. Nanosci.*, **6**(3), 682-685 (2009).

5. Youness R.A., Taha M.A., Ibrahim M.A.; Effect of Sintering Temperatures on the In Vitro Bioactivity, Molecular Structure and Mechanical Properties of Titanium / Carbonated Hydroxyapatite Nanobiocomposites, *J. Mol. Struct*., **1150**, 188-195 (2017).

6. Abdelsalam H., Elhaes H., Ibrahim M.A.; First principles study of edge carboxylated graphene quantum dots, *Physica B*, **537**, 77-86 (2018).

7. Grenni P., Caracciolo A.B., Mariani L., Cardoni M., Riccucci C., Elhaes H., Ibrahim M.A.; Effectiveness of a new green technology for metal removal from contaminated water, *Microchem. J.*, **147** 1010-1020 (2019).

8. Zhang K., Yang W., Yin X., Chen Y., Liu Y., Le J., Xu B.; Amino acids modified konjac glucomannan as green corrosion inhibitors for mild steel in HCl solution, *Carbohyd. Polym.*, **181**, 191-199 (2018).

9. Majumder S., Mishra I., Subudhi U., Varma S.; Enhanced biocompatibility for plasmid DNA on patterned TiO_2 surfaces, *Appl. Phys. Lett.*, **103**, 063103 (2013).

10. Gray H.B., Winkler J.R.; Electron transfer in proteins, *Annu. Rev. Biochem.*, **65**, 537-561 (1996).

11. Deisenhofer J., Norris J.R. (eds.); The Photosynthetic Reaction Center II, p.500, Academic Press, New York (1993).

12. Gu Q., Cheng C., Conela R., Suryanarayanan S., Anabathula S., Dai K., Haynie D.T., Nanotechnology, v. 17, R 14 (2006).

13. http://m-protect.ru/wiki/index.php?title

14. Nanoelectronics and nanobioelectronics http://nano.86sch5.edusite.ru/p17aa1.html

15. Doroshkevich A.S., Danilenko I.A., Konstantinova T.E., Glazunova V.A., Sinyakina S.A.; Diagnosis of nanopowder systemsbased on zirconia by transmission electron microscopy, *Electron Microscopy and Strength of Material*, **13**, 151-159 (2006).

16. http://www.abc.chemistry.bsu.by/vi/analyser/.

17. Kholmurodov K. (Ed.); Molecular Simulation Studies in Material and Biological Sciences, International Workshop, Nova Science Publishers Ltd., 196p., ISBN: 1-59454-607-x (2007).

18. Kholmurodov K. (Ed.), Molecular Simulation in Material and Biological Research, Nova Science Publishers Ltd., 155p., ISBN: 978-1-60741-553-4 (2009).

19. Kholmurodov K. (Ed.), Molecular Dynamics of Nanobistructures, Nova Science Publishers Ltd., 210p., ISBN: 978-1-61324-320-6 (2011).

20. Kholmurodov K. (Ed.), Models in Bioscience and Materials Research: Molecular Dynamics and Related Techniques, Nova Science Publishers Ltd., 219p., ISBN: 978-1-62808-052-0 (2013).

21. Brooks B.R., Bruccoleri RE., Olafson B.D., States D.J., Swaminathan S., Karplus M., CHARMM: A program for macromolecular energy, minimization, and dynamics calculations, *J. Comp. Chem.*, **4**, 187-217 (1983).

22. Case D.A., Cheatham T.E., Darden T., Gohlke H., Luo R., Merz K.M., Onufriev A., Simmerling C., Wang B., Woods R.J.; The Amber Biomolecular simulation programs, *J. Comp. Chem.*, **26**(16), 1668-1688 (2005).

23. Smith W., Forester T.R.; DL_POLY_2.0: A general-purpose parallel molecular dynamics simulation package, *J. Mol. Graph.*, **14**, 136-141 (1996).

24. Smith W., Forester T.R., Todorov I.T.; The DL POLY 2 User Manual, STFC Daresbury Laboratory Daresbury, Warrington WA4 4AD Cheshire, UK, Version 2.19, April (2008).

25. Kholmurodov K. (Ed.); Computational Materials and Biological Sceinces, Nova Science Publishers Ltd., 208p., ISBN: 978-1-63482-541-2 (2015).

26. Kholmurodov K.T. (Ed); Computer Design for New Drugs and Materials. Molecular Dynamics of Nanoscale Phenomena, Leading Scientist, Frank Laboratory of Neutron Physics, Joint Institute of Nuclear Research, Dubna, Moscow Region, Russia, ISBN: 978-1-53612-082-0, Nova Science Publishers, New York, 231 p. (2017).

27. Rajendran A., Endo M., Hidaka K., Sugiyama H.; Direct and Real-Time Observation of Rotary Movement of a DNA Nanomechanical Device, *J. Am. Chem. Soc.*, **135**(3), 1117–1123 (2013).

28. Mao C., Sun W., Shen Z., Seeman N.C.; A nanomechanical device based on the B–Z transition of DNA, *Nature*, **397**(6715), 144-146 (1999).

المحاكـــاة الدينـــاميكيـــة الجزيئيـــة للضـــرر الإشعـــاعي للحمض النـــووى وســـلوك التشـكل علي سطح ثاني أكسيد الزركونيوم النانومتري

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[٢] المركز الدولي للفيزياء النووية - دوبنا- الاتحاد الروسي.
[٣]جامعه دوبنا- دوبنا- الاتحاد الروسي.
[٤] المعهد الوطني للتقنية - باتنه- الهند.
[٥] قسم الطيف - المركز القومى للبحوث -٣٣ شارع البحوث - ١٢٦٢٢ الدقى - الجيزة - مصر.

يهدف هذا البحث إلي إجراء دراسة معقدة لعمليات تثبيت وتشكل الحمض النووي علي سطح الجزيئات المتناهية الصغر لثاني أكسيد الزركونيوم قي الابعاد النانومترية.

إن المركبات النانومترية للحمض النووي (DNA) و جزيئات ثاني أكسيد الزركونيوم المتناهية الصغر علي هيئة جسيمات نانومترية أو شرائح ذات حجم نانومتري تم دراساتها بإستخدام المحاكاة الديناميكية الجزيئية ، الطرق الطيفية و المتكاملة بما في ذلك الفيزياء النووية.

ولقد تم دراسه تفاعل الحمض النووي (DNA) المذاب في الماء مع سطح الجسيمات النانومترية لثاني أكسيد الزركونيوم بإستخدام أمكانيات المحاكاة الديناميكية المكونة من هجين الديناميكا الكلاسكية وكيمياء الكم. ولهذا الغرض تم إعداد سلسلة من النماذج المختلفة لمحاكاة مختلف الأحتمالات لتغييرالشحنات علي سطح الحمض النووى. ولقد تم إدخال تغيير في شحنات ذرتي الفوسفور (P_a & P_b) الموجودتان في منتصف الحمض النووي (DNA) ولقد قمنا بتقدير التغيرات الموضعية للمسافة بين ذرتي الفوسفور في الحمض النووي والأكسجين الموجود في الجسيمات النانومترية في المركبات المكونة من [DNA(Pa ,Pb) - ZrO2 (O)].

كما يهدف هذا العمل إلي تطوير فاعلية الأرتباطات الغير متجانسة مثل الجزيئات البيولوجية والعوازل واسعة النطاق. وهذة الأرتباطات الغير متجانسة موجهة للأستخدام في مجالات مثل الألكترونيات الجزيئية وخاصة إنتاج الرقائق الحيوية، ومصفوفات الذاكرة و هنسة الكمبيوتر المستقبلية.