



Original article

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**FREE ENERGY RELAXATION OF GLYCINE, TRIPTOFAN
AND ALBUMIN MOLECULES
IN THE IONIZED AQUEOUS SOLUTION: COMPUTER ANALYSIS**

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Abstract: A comparative analysis of the free energy of alanine, tryptophan and albumin protein amino acids in the aqueous solutions of sodium chloride with different concentrations (ionization degree) has been carried out using the molecular computer modeling method. Some dependences of dynamic scenarios of the behavior of the mentioned energy on the concentration of ionizing reagent (the dissociating salt) in the solutions were obtained. Such information can be applied when designing the hybrid micro and nanoelectronic devices with built-in biomolecular objects, e. g. biochemical sensors, devices with microflow of liquids, for the molecular film preparation technology, etc.

Keywords: proteins, peptides, hybrid biomolecular electronics, computer modeling

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КОМПЬЮТЕРНЫЙ АНАЛИЗ РЕЛАКСАЦИИ СВОБОДНОЙ ЭНЕРГИИ МОЛЕКУЛ ГЛИЦИНА, ТРИПТОФАНА И АЛЬБУМИНА В ИОНИЗОВАННОМ ВОДНОМ РАСТВОРЕ

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Аннотация. Методом компьютерного молекулярного моделирования осуществлен сравнительный анализ динамики свободной энергии аминокислот аланина, триптофана и белка альбумина в водных растворах хлорида натрия различной концентрации (степени ионизации). Получены зависимости динамических сценариев поведения указанной энергии от концентрации ионизирующего реагента (диссоциирующей соли) в растворах. Такие сведения можно использовать при разработке гибридных микро- и нанoeлектронных устройств с встроенными биомолекулярными объектами, например биохимических сенсоров, приборов с микропотоками жидкостей, технологии приготовления молекулярных пленок и т. п.

Ключевые слова: белки, пептиды, гибридная биомолекулярная электроника, компьютерное моделирование

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Introduction

The characteristics of hybrid micro and nanoelectronic devices with built-in biomolecular objects depend, similar to living systems, on the specific configurations of the structure, dynamics and function of molecules and their ensembles. In particular, the crucial factors are biomolecular conformation, energy, dipole moment and their evolution for particles (e.g., proteins and peptides associated with solids and solutions). Data on the dissipation of molecular energy in ionized solutions serves for developing electronic devices with liquid microflows, biochemical sensors, technologies for preparing molecular films, etc. Computer simulations and calculations of free energies of molecules are performed in many of the latest studies, in particular, to predict the probability of a certain conformation evolving [1–3]. Conformational variations are accompanied by correlated changes in the dipole moment and total energy of a molecule or molecular cluster [4–6].

The free energy landscapes characterizing the amplitude and timescale of the motions of biomolecules and biomolecular clusters during their spontaneous relaxation in aqueous solution are used to parametrize the states of organic objects built into hybrid electronic devices [7]. Similar data were obtained, for example, for subpicosecond vibrational dynamics of the dipole moment for some polypeptides measured by spontaneous Raman spectroscopy [6, 8, 9]. However, the fundamentally important relationship between dipole oscillations and the total free energy of molecules was not established. Free energy is the key thermodynamic quantity because the change in free energy associated with a molecular process determines whether the process can occur spontaneously under the given thermodynamic boundary conditions. In practice, the values of free energy make it possible to compare the results of experimental studies with the data of computer simulation [10–12]. Research into dynamic relaxation of free energy of biomolecules and their clusters in aqueous media can yield the most complete data on the structure and properties of molecular ensembles [13, 14].

The molecules and molecular clusters of glycine, tryptophan and albumin peptides were chosen in our paper based on similar available studies suitable for comparative analysis, as well as known promising applications in hybrid electronic devices. For instance, [15,16] consider studies of glycine peptide for various applications, including biomedical. Mechanisms of ion conductivity in organic compounds, including albumin, are given in [17], arguing that albumin shows potential for developing biomolecular electronics devices. It was confirmed in [18, 19] that doping with tryptophan noticeably increases the electrical conductance of the alanine molecule, which makes tryptophan an attractive candidate for biomolecular electronics.

The numerical computations in this paper were performed to obtain and analyze the dependences of free energy on amplitude and timescale for molecules and molecular clusters of glycine, tryptophan, and albumin in aqueous solutions with various concentrations of ionizing dissociating salts. The data obtained allowed to construct the corresponding model representations.

Our findings can be used for developing hybrid micro and nanoelectronic devices with built-in biomolecular objects, for example, biochemical sensors, devices with liquid microflows, technologies for preparing molecular films, etc.

Models for computer study

Visual Molecular Dynamics (VMD) software was used to generate the molecular models. It is a computer program designed for molecular modeling and visualization of molecular systems. It is also used for computer studies of the free energy of large conformationally mobile molecules.

The model of a molecule or cluster for each peptide and protein from the experimental set consisted of one or four molecules placed in a periodic water box. The size of the box varied from 50 to 120 Å (depending on the size of protein molecules and their number). The distance from the end molecule to the box boundary was 15 Å in all computational systems. The molecules were dissolved via the TIP3W model corresponding to three atoms of a water molecule at three points of interaction with the molecule. Such models provide high computational efficiency in many applications for simulating molecular dynamics. However, the water model we used was also implemented in the CHARMM force field. The difference lies in the Lennard–Jones parameters: unlike TIP3, the CHARMM version of the model assigns these parameters to hydrogen atoms in addition to the oxygen parameters in the water molecule [20, 21]. This water model is adopted in most of the available studies known to us.

The free energies of a molecule or cluster in aqueous solution were calculated by the Free Energy Perturbation (FEP) algorithm in the Visual Molecular Dynamics (VMD) program. The FEP algorithm is based on the laws of statistical mechanics; it is used in computational chemistry to determine free energy from molecular dynamics data. The algorithm determines the energy difference between two states of the system at each instant in time, which allows building a dynamic scenario for the evolution of the processes in the system. Since the calculations were performed at constant pressure, free energy is associated with Gibbs energy.

An option to add ions at a certain concentration $n[\text{mol/l}]$ in the water box was used to model the procedure generating the salt solutions in the program. Ion concentrations in aqueous solutions were varied in the simulation by introducing NaCl salt ions with a minimum distance of 5 E between the ions. Similar methods were adopted in our earlier experiments [22, 23]. Na^+ and Cl^- ions were added to change the salt concentration from $1.71 \cdot 10^{-4}$ to 1.71 mol/l, which corresponded to a mole fraction range from 0.001 to 10%. In this case, the maximum number of ions per molecule in the water box was about 3200. Since the albumin protein molecule is much larger than the tryptophan or glycine molecules, it accounted for a relatively higher number of salt ions in the water box.

Molecular modeling was carried out with a CHARMM27 force field applied, using the NAMD (Nanoscale Molecular Dynamics) package. NAMD runs molecular dynamics simulations implemented in the Charm++ parallel programming paradigm, which has high parallelization efficiency and is often used for modelling large systems. Periodic boundary conditions were imposed with the cutoff (for non-bonded interactions with switching) starting from 9 E and up to 12 E. The instant in time when equilibrium was reached in the system was simulated by setting the conditions for minimizing the energy and stabilizing the conformational state of molecules.

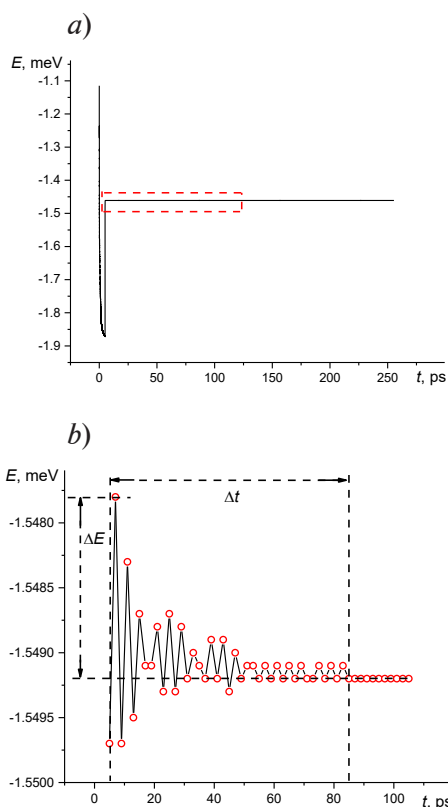


Fig. 1. Energy landscape of the albumin molecule in aqueous solution of NaCl with a concentration of 0.15 mol/l at time intervals of 300 ps (a) and 110 ps (b). The graph in Fig. 1,b corresponds to the region enclosed by a rectangle in Fig. 1,a (energy relaxation process); ΔE is the initial excess energy of the molecule, Δt is the time interval in which the energy reaches a steady state



Minimizing the energy yielded stable conformational states of molecules necessary for further analysis when the molecules would be ‘placed in a solution’.

The Langevin equation was used for minimizing the energy and calculating the relaxation of molecular objects:

$$m_i \frac{d^2 x_i(t)}{dt^2} = F_i \{x_i(t)\} - \gamma_i \frac{dx_i(t)}{dt} m_i + R_i(t), \quad (1)$$

where x_i , m, is the object coordinate; t , s, is the time; γ_i is the friction coefficient; m_i , g, is the particle mass; $\gamma_i m_i$, g, is the damping coefficient of the system; F_i , N, is the force experienced by a particle exposed to an electric field (for example, generated by ions); R_i , N, are the random forces acting on the particle.

The Langevin method made it possible to calculate the kinetic energy of the system while simultaneously monitoring the temperature of the molecular object and the pressure of the environment. Fig. 1 shows the dependence of total energy on time for an albumin molecule in a water-salt solution with a NaCl concentration of 0.15 mol/l. The molecule energy was minimized in the initial time interval lasting about 5 ps (Fig. 1, *b*). Apparently, the process of energy relaxation is triggered right after energy minimization is started. It is assumed that oscillations of the molecular cluster occur in this interval, when the excitation energy of the molecules is imparted to the solution.

The energy reaches an average steady-state level in a time Δt ; meanwhile, the initial excess energy of the molecule relaxes by ΔE , which is approximately equal to the difference between the final steady-state and initial energy values.

The total energy of a molecule is the sum of kinetic and potential energy

$$H(p, r) = K(p) + V(r), \quad (2)$$

where p is the total momentum, r are the generalized coordinates.

The kinetic energy follows the expression

$$K(p) = \sum_{i=1}^N \frac{p_i^2}{2m_i}, \quad (3)$$

where p_i are the particle momenta, N is their number.

Kinetic energy is mainly represented by the rotation of peptide groups, while potential energy is the sum of various components.

The largest contribution to the potential energy is made by the electrostatic potential

$$U_{elec} = \varepsilon_{14} \frac{C q_i q_j}{\varepsilon_0 r_{ij}}, \quad (4)$$

where $r_{ij} = \|\mathbf{r}_j - \mathbf{r}_i\|$, m, gives the distance between a pair of atoms; q_i, q_j, C , are the charges on the corresponding atoms; ε_{14} is the dimensionless scale factor, $\varepsilon_{14} = 1$ (with rare exceptions, see below); C is the Coulomb constant, $\tilde{N} = 8.9888 \cdot 10^9 \text{ N} \cdot \text{m}^2 / \text{C}^2$; ε_0 is the vacuum permittivity, $\varepsilon_0 = 8.8542 \cdot 10^{12} \text{ F/m}$.

The quantities C and ε_0 are fixed for all electrostatic interactions. The value of the parameter ε_{14} is equal to 1, except for the modified 1–4 interaction, where a pair of atoms is separated by a sequence of three covalent bonds (as a result, atoms can also participate in the interaction with the torsional angle); $\varepsilon_{14} = \varepsilon$ in this case for a fixed value of vacuum permittivity lying in the range $0 \leq \varepsilon \leq 1$ [22].

The salt concentration was varied in the range from 0.001% to 10%, which corresponds to $1.71 \cdot 10^{-4} - 1.71 \text{ mol/l}$.

The obtained energy landscapes of molecules and clusters were processed by the fast Fourier transform to obtain the frequency spectra.

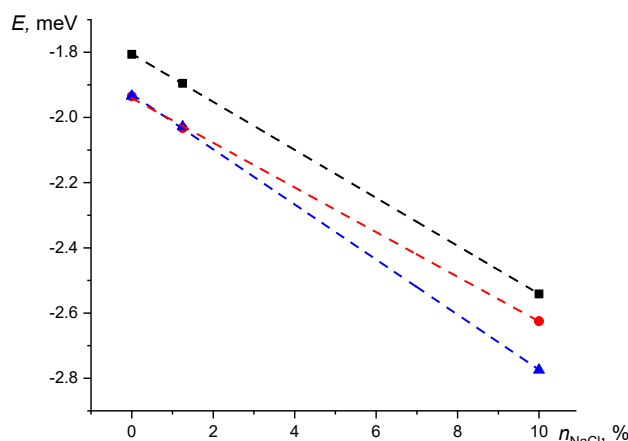


Fig. 2. Energy depending on the concentration of the water-salt solution at the time $t_0 = 3$ ns for tryptophan, glycine and albumin molecules (blue, red and black lines, respectively)

Results and discussion

Regions of initial relaxation from ΔE (see Fig. 1,*b*) appearing to be oscillations with a decreasing amplitude lasting up to approximately 250 ps, and longer (lasting up to 10 ns and more) quasi-harmonic oscillations with a small amplitude were observed on the curves describing the dependence of energy on amplitude and timescale. The amplitude of such quasi-harmonic oscillations was much less than the values of the total energy, allowing to consider the mechanisms for the stabilized equilibrium (average) values.

Changing the ion concentration in the solution led to a change in the relaxation time. Fig. 2 presents an overview for the steady-state values of total energy for tryptophan, glycine, and albumin molecules depending on the concentration of NaCl salt in the solution at a time of 3 ns. Evidently, the total steady-state energy of the molecule decreases with increasing salt concentration (the refined characteristics are given below in Fig. 3).

Fig. 3 shows examples of energy dependences on amplitude and time for three types of molecules during the intervals of 0–0.1 and 3.00–3.01 ns. Apparently, the initial process of energy relaxation is characterized by damped oscillations, while quasi-harmonic oscillations of small amplitude are accompanied by frequency beats.

Long-term scenarios of the energy dependences on amplitude and time were calculated for a period up to 100 ns and a sampling step of 1 ps for subsequent Fourier analysis of these dependences (using the OriginPro software). As an example, Fig. 4 shows the Fourier spectrum for such an energy landscape of a glycine molecule in aqueous solution of sodium chloride with a concentration of 1.25% over a time interval from 5 to 65 ns. A region with an increased spectral density was detected in the spectrum near 0.44 THz, which approximately corresponds to the dependence in Fig. 3,*c*.

In other cases, i.e., at lower and higher concentrations of sodium chloride, the frequency spectra for glycine and other molecules, had a more complex shape. The patterns discovered require additional analysis, which is beyond the scope of this study.

Fig. 5,*a,b* shows the dependences of steady-state energies on the salt concentration in systems containing both one molecule and a cluster of four molecules. It can be seen that the given dependences behave almost similarly, i.e., the system is insensitive to the clustering of molecules.

The dependences of energy relaxation time (Fig. 5,*c,d*) can be approximated by straight lines, which allows to conclude that the decrease in the amplitude bears an exponential character. The exponents apparently differ for different types of molecules and their clusters.

Calculations indicate that the initial nonequilibrium free energies of a single molecule and a molecular cluster exhibit a trend towards fluctuating decrease during dissipation, i.e., during the time interval when the cluster primarily loses energy to the solution via relaxation, with the energies subsequently reaching a quasi-stationary level as a balance of energy fluxes from the cluster to the solution and vice versa is established.

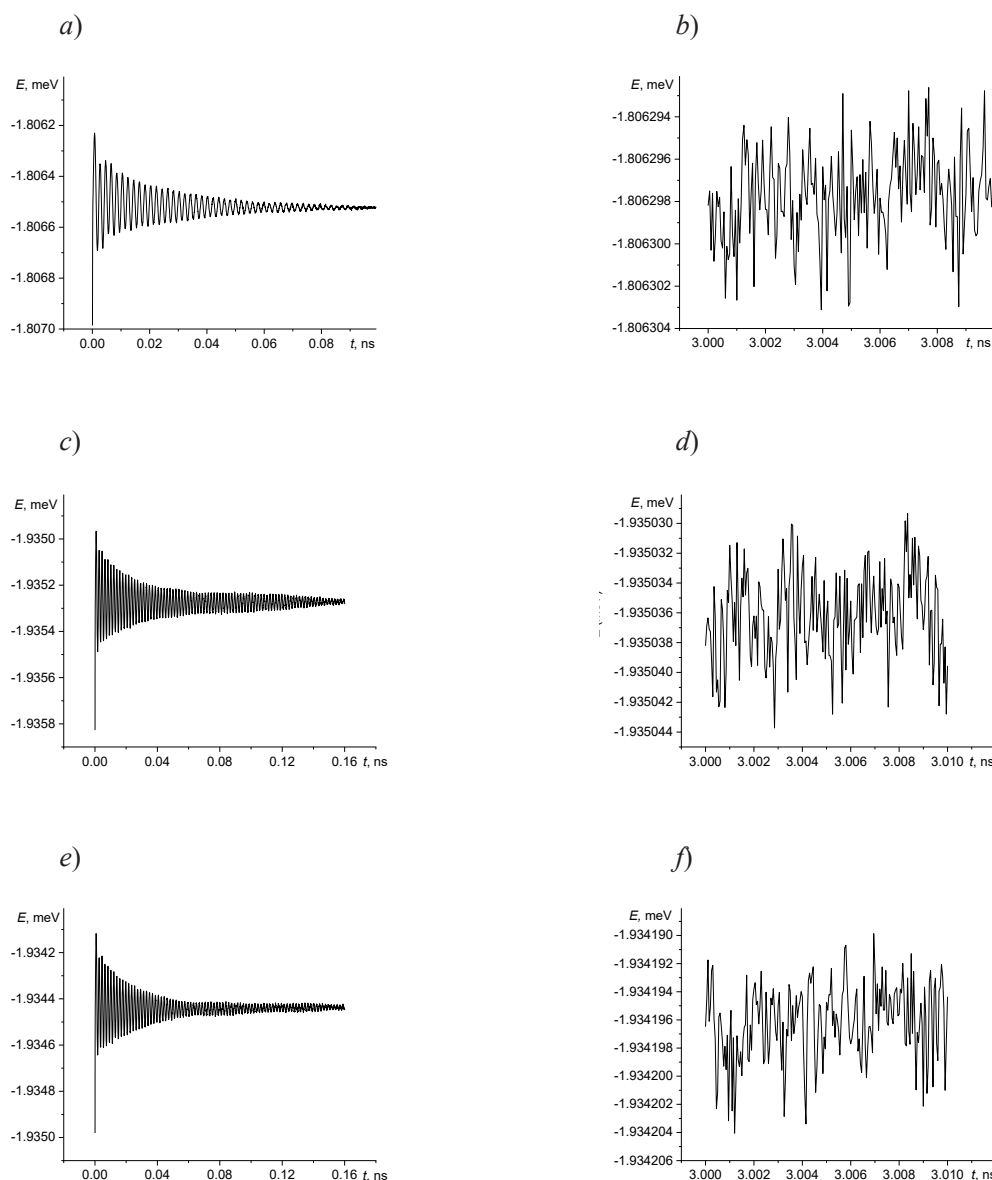


Fig. 3. Energy landscapes for albumin (*a, b*), glycine (*c, d*) and tryptophan (*e, f*) molecules in water-salt solutions with a concentration of 0.001% during two time intervals

The oscillatory energy of molecules or clusters is pumped into the oscillations of ions produced during the dissociation of salt. The total energy of the cluster is much higher than the relaxation energy; this means that the kinetic component of energy is mainly engaged in pumping.

The time it takes for energy to relax to a quasi-stationary state depends on the salt concentration. As the salt concentration increased, the energy losses of the molecule occurred faster than at an initially lower salt concentration. Energy relaxation that occurs with slow aperiodic oscillations is similar to the relaxation of a dissipative dynamic system with low electrical conductivity and increased ‘friction’.

The observed effect likely corresponded to a decrease in the electric field strength above the surface of each molecule due to a shift in the pH towards the alkaline region and a corresponding increase in electrical conductivity of the water-salt solution.

The relaxation of free energy detected in a molecular cluster indicates that electrodynamic factors play a significant role in the biomolecular processes considered.

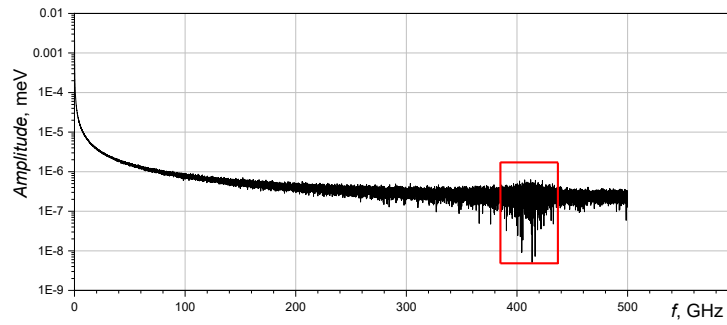


Fig. 4. Fourier spectrum for the oscillation frequency of the glycine molecule in water-salt solution with a concentration of 1.25%. The red box highlights a region with increased spectral density near 440 GHz

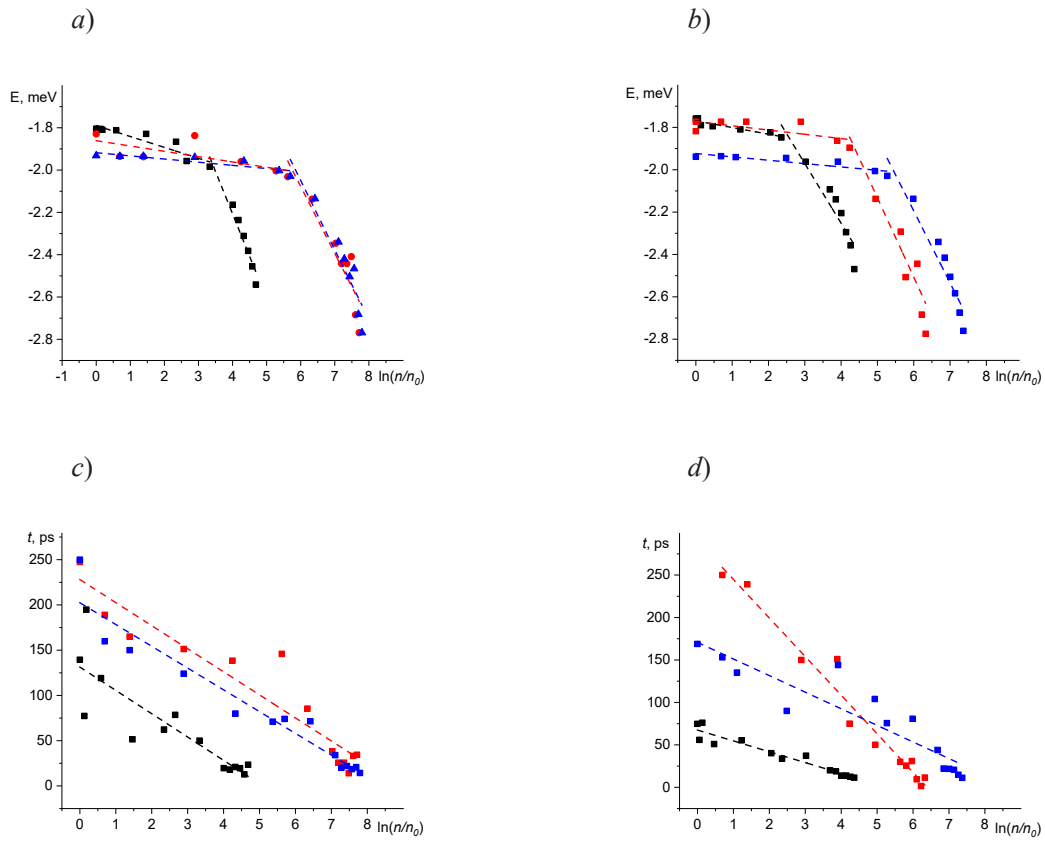


Fig. 5. Dependences of energy (*a,b*) and relaxation time (*c,d*) on the concentration of NaCl water-salt solution for single molecules of tryptophan, albumin and glycine (*a,c*), and clusters of 4 molecules (*b,d*). The line colors correspond to those in Fig. 2



Conclusion

Numerical simulations were used for comparative analysis of the free energy landscapes of alanine, tryptophan and albumin amino acids in water-salt solutions with different concentrations (degrees of ionization). Data were obtained for the dependence of dynamic scenarios of free energy and its relaxation time on the concentration of ionized dopants of dissociating salts in the solution. We have confirmed that the energy and spectral characteristics of molecules in water-salt solutions can be controlled by changing the ionization degree of the solutions. These data can be used for developing hybrid micro- and nanoelectronic devices with built-in biomolecular objects, for example, biochemical sensors, devices with liquid microflows, technologies for preparing molecular films, etc.

The results were obtained using the resources of the Supercomputer Center at Peter the Great St. Petersburg Polytechnic University (www.scc.spbstu.ru).

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