Simulation of Coulomb-coupled, Protein-based Logic

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Abstract:

In this theoretical work, I investigate photoswitchable proteins as possible building blocks of computing, and signal processing architectures of the future. Coulomb-coupled, photon-pulse controlled macromolecular arrays are proposed and explored with the aid of a simple, mixed quantum-classical, nanoelectromechanical model. I show chains for digital signal propagation, and possibly universal logic gates, therefore computing architectures can be constructed from such proteins. Furthermore, I explore the basic molecular properties needed for their realization, and I show that photoswitchable proteins are possible candidates for this purpose.

Keywords: *nanotechnology, nanoelectronics, molecular electronics, photoswitchable protein.*

1. Introduction

The continuously increasing need for improving computer power results in a steady increase of the number of electronic components in microprocessors (Moore's law). In order to realize fast, low-cost, low power consuming and dissipating nanometre-size electronic devices, new concepts must be explored by taking advantage of effects arising on the nanometre-scale. Since the size of such devices is expected to eventually reach the molecular level, an emphasis must be given on the investigation and implementation of novel computing architectures based on molecules.

Since Coulomb forces are the strongest intermolecular forces in molecular arrays, Coulomb-coupling [1] is a possible way for the integration of molecule-based electronic elements. The concept of photon-pulse driven, polymer-like signal processing arrays has been presented previously [2], and their advantages have been discussed in the case of two-state quantum systems with mechanical vibration in one variable [2]-[4].

Since proteins are low-cost macromolecules that can be ordered in self-assembled monolayers, and can be engineered to provide desirable properties, they are possible candidates for the realization of molecular computers. It has been demonstrated in the case of Dronpa that such molecules can be reversibly photo switched between states even at the single-molecule level [5].

In this paper, I extend the model presented in [2] to be suitable for the simulation of dipole-dipole coupled photoswitchable proteins placed next to each other. Furthermore, I simulate digital signal propagation in a one-dimensional chain consisting of closely placed proteins (Fig. 1). I show that such photoswitchable proteins have potential advantages in molecular computing.

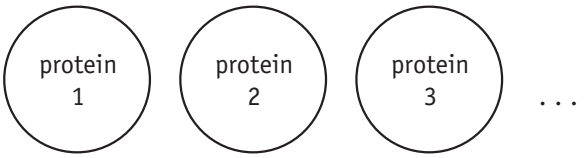

Fig. 1. Diagram of a chain arrangement of closely placed proteins.

2. Modelling

For the simulations I used a simple quantum-classical dynamical model based on [2], where both molecular electron and proton transfers are taken into account. For the sake of simplicity I assumed that the molecule can be described as a two-state system, and I presupposed that the potential energy surfaces (PES) as the function of the reaction coordinate, and the damping parameters are known. The Hamiltonian matrix of the molecule depends on the reaction coordinate q:

$$\mathbf{H} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} = \begin{pmatrix} E_1(q) & G(q) \\ G(q) & E_2(q) \end{pmatrix}. \tag{1}$$

The equations describing the coupled nanoelectronic and nanomechanic behaviour of the molecules assuming the simplest dissipation model are the following:

$$\frac{d\vec{\lambda}(t)}{dt} = \mathbf{\Omega}\lambda(t) - \frac{1}{\tau}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}\lambda(t) + \frac{1}{\tau}\begin{pmatrix} 0 \\ 0 \\ 2\tanh\dfrac{\Delta E}{k_B T} \end{pmatrix} \tag{2}$$

$$\frac{d}{dt}q(t) = \frac{1}{M}p(t) \tag{3}$$

$$\frac{d}{dt}p(t) = \left\langle \Psi \right| - \frac{\partial}{\partial q}\left(V_{nn} + V_{en}\right)\left| \Psi \right\rangle - \alpha p(t), \tag{4}$$

where $\vec{\lambda}(t) = \left[\lambda_1(t), \lambda_2(t), \lambda_3(t)\right]$ is the three-dimensional quantum-coherence-vector, V_{nn}, V_{en} are the nucleon-nucleon and electron-nucleon potential energies (they can be determined from the PES), respectively. The aforementioned equations were used in [2] for the simulation of two-state quantum systems with one-dimensional nuclear vibration, therefore there the reaction coordinate, q represented the distance between the nuclei (bond length), p corresponded to the momentum, and M described the mass of the nucleus. In this study q is used in a more general sense, since the choice of the reaction coordinate depends on the nature of the reaction (e.g. if

q is the bond length then p is the momentum, M is the mass of the atom, if q is chosen to be the bond angle then p is the angular momentum, M is the moment of inertia), which depends on the choice of the photoswitchable protein under investigation. The α parameter characterizes the mechanical, τ represents the electronic relaxation. The

$$\mathbf{\Omega} = \begin{pmatrix} 0 & -H_{22}+H_{11} & -j(H_{12}^{*}-H_{12}) \\ H_{22}-H_{11} & 0 & -H_{12}-H_{12}^{*} \\ j(H_{12}^{*}-H_{12}) & H_{12}+H_{12}^{*} & 0 \end{pmatrix} \quad (5)$$

matrix is the Bloch matrix. Since in our case the internal molecular dynamics cannot be described using solely the adiabatic approximation, surface hopping [6] between the two electronic states was incorporated in the model as well. According to Rabi's theory, the external electromagnetic field (photon pulse) interacts with the dipole moment of the molecule adding a time-varying component to the off-diagonals of H in equation (1). Coulomb-coupling with the neighbouring molecules changes the difference between the energy levels of the molecule:

$$\Delta E = \Delta E_0 + \frac{\Delta\mu}{4\pi\varepsilon_0}\sum_i \frac{\mu_i}{d_i^3}, \quad (6)$$

where ΔE and ΔE_0 are the differences between the two energy levels with and without the influence of the neighbours, respectively, $\Delta\mu$ is the transition dipole moment of the molecule, μ_i is the dipole d_i moment of the i-th neighbour, and di is the distance between the molecule and its i-th neighbour.

3. Results and discussion

The energy (frequency) of the photon pulse required to switch a photoswitchable protein from state 1 to state 2 usually significantly differs from that of the pulse, which switches it back to state 1 (selective switching). It has been already shown in the case of Coulomb-coupled, two-state molecules with one-dimensional nuclear vibration that such selective switching permits the realization of universal logic gates (Fredkin gate, and majority gate combined with inverting molecules) [2]. Since photoswitchable proteins can be switched selectively as well, they also permit the realization of such logic gates. In the following I will discuss the potentials of such proteins in the realization of computing and signal processing architectures with the aid of our model.

3.1. Pulse-driven photoswitchable protein chain

The following example demonstrates the process of loading a bit on the second protein of a chain consisting of identical photoswitchable proteins (Figure 2) similarly to [2] that used the same example structure in the case of diatomic molecules. The potential energy curves of the reversibly photoswitchable protein are displayed in Figure 2(a). The molecule has two stable ground state configurations (state 1, state 2), the two states have different dipole moments (μ_1=500 Debye, μ_2=1000 Debye), it can be switched to the excited states of the two different configurations by photons with different energies (in the example ΔE_1=2 eV, ΔE_2=3 eV). The transition dipole moments were set to $\Delta\mu_1$=$\Delta\mu_2$=20 Debye during the simulation, and the distance between proteins was set to 3 nm. All of these data are within realizable domains. The difference between the two energy levels of the protein depends on the dipole moments of the neighbouring molecules (see equation (6)), and since the dipole moments of the two states of a photoswitchable protein can differ significantly, the states of the neighbours can strongly influence the photon frequency required to switch the corresponding protein, thereby improving the selective nature of the switching, which is a major advantage of such macromolecules. In the case of other kinds of molecules, where only the transition dipole moments between ground and excited states play a role in switching, the coupling effect is much smaller, since the transition dipole moments are usually significantly smaller than the dipole moment difference between the two stable states of photoswitchable proteins. If I assume that in the beginning all of the proteins are in state 1, the process is the following: first the entire chain is subjected to pulse 1 with frequency ω_1^1 (the subscript shows the state of the molecule, the superscript is '1' or '2', if the neighbour(s) of the protein is in state 1 or state 2, respectively) that switches the first member of the chain to state 2. Then the chain is irradiated by pulse 2 with ω_1^{12} that switches the second protein to state 2. The last pulse with ω_2^2 switches the first molecule back to state 1. The demonstration of the photoswitchable protein majority and Fredkin gates is straightforward by taking into account the afore-presented simulation and the discussions in [2].

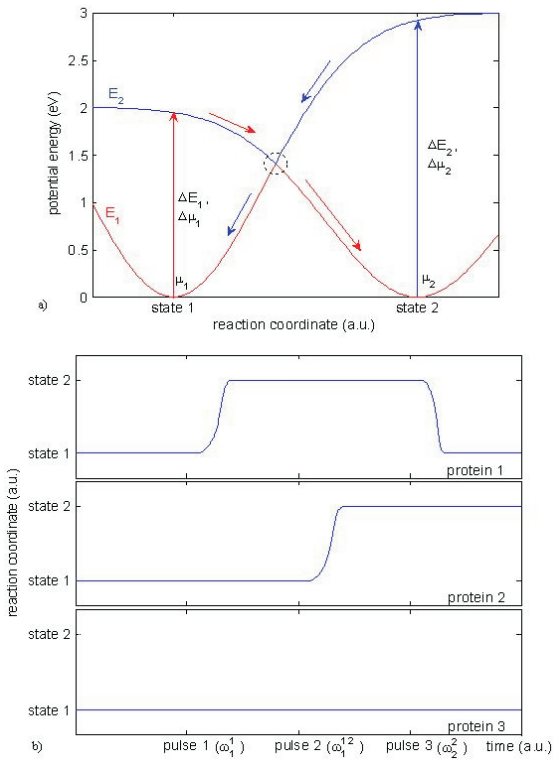

Figure 2. Loading a bit to the second protein of a chain consisting of identical proteins. a): Potential energy curves of the protein. The red and blue arrows show the reaction paths from state 1 to state 2 and vice versa, respectively. The dashed circle highlights the place, where surface hopping occurs between the two states. b): Three subsequent photon pulses load a bit onto the second protein.

3.2. Other energy-level arrangements

Figure 3(a) displays an arrangement in which the influence of the states of the neighbours on the energy level difference of the corresponding molecule can be further improved. Let us assume that state 2 of molecule B is originally not stable, and the dipole moment of state 1 (μ_1) is greater than that of state 2 (μ_2). The influence of molecule A on the energy difference between the two states of B is described by

$$\Delta E = \Delta E_0 - \frac{1}{4\pi\varepsilon_0}\frac{\mu_A}{d_{AB}^3}\left(\mu_1 - \mu_2\right), \tag{7}$$

where ΔE_0 is the energy difference without the influence of molecule A, d_{AB} is the distance between the molecules. Since ΔE depends on the state of molecule A, by properly choosing the parameters of the molecules, a stable state 2 can be induced if molecule A is switched from state 1 to state 2, since the dipole moment of state 2 of molecule A is greater than that of state 1, thereby lowering the energy of state 2 of molecule B with respect of state 1. Note that in this case molecule B can be switched from state 1 to state 2 only if molecule A is in state 2. A main advantage of this arrangement is that the influence of the states of the neighbours on the energy levels of the protein is even stronger than in the previous case (section 2.1), since the energy difference between the states of molecule B depends on the product of μ_A and μ_B, where both μ_A and μ_B can be significantly higher than the transition dipole moment in equation (6).

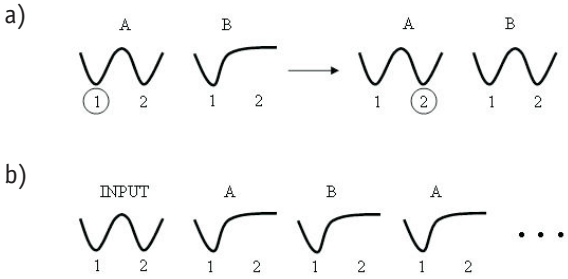

Figure 3. a) illustrates the effect of inducing a stable state 2 in molecule B by switching molecule A to state 2. b) displays the energy levels of molecules in a one-dimensional molecular chain. Only the ground-state energy levels are shown.

This kind of arrangement also permits signal propagation and the realization of logic gates. Figure 3(b) shows the ground-state energy levels of a molecular chain consisting of an input protein, and two other molecules with different parameters. The sequence of propagating a bit along the chain by subsequent photon pulses is the following: the input molecule is switched to state 2, which induces a stable state 2 in the second molecule in the chain; then the second molecule is switched to state 2, which induces a stable state 2 in the third molecule; the third molecule is switched to state 2, a stable state 2 is induced in the fourth molecule; the input molecule is switched back to state 1; the fourth molecule is switched to state 2; the second molecule is switched back to 1, and the process goes on until the signal reaches the other end of the chain.

4. Conclusion and future outlook

In this paper, I discussed the potential of photoswitchable protein molecules in the realization of macromolecular computing, and digital signal processing arrays. For the simulations I used a simple quantum-classical nano-electromechanical model. Such proteins are potential candidates of future nanometre size computing architectures since they are cheap, can be assembled in monolayers, can be engineered to provide desired properties. Furthermore, they can provide stronger influence on each other during Coulomb-coupling.

The authors hope that this study encourages further experimental studies needed for the realization of such computing architectures. Future studies should include the identification of already existing or artificially developed proteins with the desired properties as well as the application of nanotechnology for the fabrication of these structures.

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References

[1] Porod W., Lent C.S., Bernstein G.H., Amlani I., Snider G. I., Merz J.L., "Quantum-dot cellular automata computing with coupled quantum dots", *International Journal of Electronics,* vol. 23, no. 5, 1999, pp. 549-590.

[2] Csurgay Á.I., Porod W., Rakos B., "Signal processing by pulse-driven molecular arrays", *Int. J. Circ. Theor. Appl.*, vol. 31, 2003, pp. 55-66.

[3] Rakos B., Csurgay Á. I., Porod W., "Recovering pure states in two-state quantum systems", *Superlattices and Microstructures*, vol. 34, 2003, pp. 503-507.

[4] Rakos B., Porod W., Csurgay Á. I., "Computing by pulse-driven nanodevice arrays", *Semicond. Sci. Technol.*, vol. 19, 2004, pp. 472-474.

[5] Habuchi S., Ando R., Dedecker P., Verheijen W., Mizuno H., A. Miyawaki, Hofkens J., "Reversible single-molecule photoswitching in the GFP-like fluorescent protein Dronpa", *Proc. Nat. Acad. Sci.*, vol. 102, no. 27, 2005, pp. 9511-9516.

[6] Tully J., Preston R., *J. Chem. Phys.*, vol. 55, 1971, pp. 562.