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Slowing down and stretching DNA with an electrically tunable nanopore in a p–n semiconductor membrane

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Abstract
We have studied single-stranded DNA translocation through a semiconductor membrane consisting of doped p and n layers of Si forming a p–n-junction. Using Brownian dynamics simulations of the biomolecule in the self-consistent membrane–electrolyte potential obtained from the Poisson–Nernst–Planck model, we show that while polymer length is extended more than when its motion is constricted only by the physical confinement of the nanopore. The biomolecule elongation is particularly dramatic on the n-side of the membrane where the lateral membrane electric field restricts (focuses) the biomolecule motion more than on the p-side. The latter effect makes our membrane a solid-state analog of the α-hemolysin biochannel. The results indicate that the tunable local electric field inside the membrane can effectively control dynamics of a DNA in the channel to either momentarily trap, slow down or allow the biomolecule to translocate at will.

Online supplementary data available from stacks.iop.org/Nano/23/255501/mmedia

(Some figures may appear in colour only in the online journal)

1. Introduction

Over the last decade nanopores have become a powerful tool for investigation of single biomolecule dynamics [1, 2] with ultra-fast and low cost DNA sequencing being one of the major goals of nanopore research [3]. To probe the physical properties of biomolecules, biological and solid-state nanopores with dimensions comparable to the diameter of a single-stranded DNA (ssDNA) cross-section (1–2 nm) are utilized [4]. In this approach, the probed molecule is forced by an applied electric field to translocate through the nanopore in a membrane that separates two compartments filled with electrolyte solution [5].

Initially, the single α-hemolysin (α-HL) channel in a lipid membrane was used as the nanopore. Later, thin solid-state membranes were also introduced, including dielectric and semiconductor membranes [6, 7] and more recently graphene-based systems [8–10]. Currently, solid-state nanopores with diameter down to ~1 nm have been created and experimentally studied, mostly via measurement of the ionic current blockades induced by the translocating biomolecule. While biological nanopores have the obvious advantage of being compatible with biomolecules [11–13], artificial nanoporous membranes provide physical stability [14, 15], precise control over the pore dimensions [16], local electrostatic potential distribution [17–19] and the promise of electrical tunability to suit the characterization needs of a particular biomolecule [17–24].

Both artificial and biological nanopores, although different in their material make-up, offer similar means of control over the biomolecule dynamics due to the largely electrostatic nature of the interaction between the nanopore membrane and the biomolecule. As such, they also face similar limitations. The typical recorded translocation time at 120 mV electrolyte bias for a DNA moving through a nanopore is of the order of 1–20 µs/nucleotide [25, 26].
This time should be increased to about 1 ms/nucleotide, to allow enough room for accurate sampling of each nucleotide [4, 27]. In addition, the secondary structure of the probed molecule interferes with the recorded signal which makes it hard to discriminate between the signals from the charge of the molecule and the secondary structure itself [11, 17, 28], indicating that the biomolecule should be stretched and slowed down even more.

In this paper, we show that these issues can be addressed during an ssDNA permeation through a nanopore in a thin semiconductor membrane made of spatially separated layers of p- and n-doped silicon (p–n-membrane). Using Brownian dynamics (BD) simulations of a ssDNA in a self-consistent membrane–electrolyte electrostatic potential from the Poisson–Nernst–Planck (PNP) approach, we show that in such a membrane, the biomolecule translocation dynamics is dramatically changed. Not only is the translocation time increased, but the polymer’s extension is much larger than when its motion is constricted only by the physical confinement of a nanopore. Moreover, the ssDNA dynamics can be electrically controlled in a broad range due to the well-known tunability of semiconductor materials.

The paper is organized as follows. Section 2 details our coupled PNP and BD approach. The results of DNA translocation simulations for different biases applied to the p–n-membrane are presented and discussed in section 3. Finally, section 4 contains a brief summary of the work and concluding remarks.

2. Method

Our simulated system is schematically shown in figure 1. The solid-state membrane consists of two 11.5 nm-thick layers of n- and p-doped Si covered by a 1 nm-thick layer of silicon dioxide (SiO2). The \( L = 25 \) nm-thick membrane is immersed in an electrolyte solution (KCl) with concentration \( C_{\text{KCl}} = 0.2 \) M corresponding to the Debye screening length \( L_D = \sqrt{kT/(2C_{\text{KCl}}e^2)} \approx 0.67 \) nm. The inner (outer) diameter of the nanopore is 2 (4) nm. Since \( L_D \) is smaller than either of the nanopore radii, this justifies the applicability of the continuum PNP approach for our membrane structure [37, 38]. The chosen nanopore parameters are well within the current experimental and technological capabilities [20]. To find the electrostatic potential distribution \( \phi(\mathbf{r}) \) generated by the membrane and the electrolyte, we solve the Poisson equation:

\[
\nabla \cdot [\varepsilon(\mathbf{r}) \nabla \phi(\mathbf{r})] = -\rho(\mathbf{r}),
\]

where \( \rho(\mathbf{r}) \) is the charge density, \( \varepsilon(\mathbf{r}) = \varepsilon_0 \varepsilon_r(\mathbf{r}) \), \( \varepsilon_r = 11.7 \) for Si, \( \varepsilon_r = 3.9 \) for SiO2, and \( \varepsilon_r = 78 \) for the electrolyte (KCl), \( \varepsilon_0 \) is the permittivity of free space. Note that the values of \( \varepsilon_r \) for Si and SiO2 are fixed while the electrolyte dielectric constant inside the pore may be different from its bulk value depending on whether or not water is excluded from the nanopore [20].

To find the electrostatic potential, the charge density \( \rho(\mathbf{r}) \) is given by:

\[
\rho(\mathbf{r}) = \begin{cases}
    e\{C_{K^+}(\mathbf{r}) - C_{Cl^-}(\mathbf{r})\}, & \text{electrolyte,} \\
    e\{\rho(\mathbf{r}) - n(\mathbf{r}) + N_D^+(\mathbf{r}) - N_A^-(\mathbf{r}) + N_{\text{surf}}(\mathbf{r})\}, & \text{membrane,}
\end{cases}
\]

where \( \rho(\mathbf{r}) \) and \( n(\mathbf{r}) \) are the concentrations of electrons and holes while \( N_D^+(\mathbf{r}) \) and \( N_A^-\mathbf{(r)} \) are the acceptor and donor densities in the semiconductor regions, respectively, \( N_D = N_A = 2 \times 10^{20} \text{ cm}^{-3} \) (this value of \( N_D = N_A \) concentration is possible to achieve in experiments [29]). \( N_{\text{surf}}(\mathbf{r}) = 4 \times 10^{20} \text{ cm}^{-3} \) represents the fixed surface charge on the membrane (in the SiO2 layer). The electrons and holes in the semiconductor regions follow Fermi–Dirac statistics [30]. Further details can be found elsewhere [18, 31–33].
Local concentrations of potassium and chloride ions, \( C_{K^+}(\mathbf{r}) \) and \( C_{Cl^-}(\mathbf{r}) \), are computed from the solution of the steady-state Nernst–Planck equations [37]:

\[
\nabla \cdot [\mu_i C_i \nabla \psi + z_i D_i \nabla C_i] = 0, \quad i = K^+, Cl^-;
\]

where \( D_{K^+} = 1.95(2.03) \times 10^{-5} \text{ cm}^2 \text{s}^{-1} \) is the diffusion coefficient, \( \mu_i \) is the mobility, \( D_i = \mu_i kT/\epsilon \), \( z_i = \pm 1 \) depending on the species charge sign. The applied electrolyte bias (in the z-direction) is 0.2 V for all simulations. Further details of this model will be given elsewhere [45].

To describe the biomolecule dynamics, we utilize the BD approach where we treat each DNA nucleotide (consisting of three sub-units—phosphate, sugar, and base) as one bead [34–36, 39], though it is in principle possible to differentiate between different types of bases via different base stacking and hydrogen bonding potentials [35]. Neglecting bead accelerations, we discretize the Langevin equations that determine the positions of beads \( \mathbf{r}_i(t) \) at time \( t \) as follows:

\[
\mathbf{r}_i(t) = \mathbf{r}_i(t - \delta t) - \nabla U[\mathbf{r}_i(t - \delta t)] \frac{\delta t}{\xi} + \sqrt{\frac{6 \delta kT}{\xi}} \mathbf{n}_i, \quad i = 1 \cdots N_b,
\]

where \( \xi = 7.5 \times 10^{-9} \text{ N s m}^{-1} \) is the viscosity of the solution, \( \delta t = 5 \text{ ps} \) is the time increment of the simulations, and \( N_b = 45 \) is the number of beads (nucleotides) in the DNA molecule, \( T = 300 \text{ K} \). The last term in this equation is due to the random force which is responsible for the stochastic motion of the beads with \( \mathbf{n}_i \) being the 3D random vector with components uniformly distributed in the interval \([-1, 1]\).

The potential energy \( U(\mathbf{r}_i) \) of the \( i \)th bead in equation (4) has several contributions:

\[
U(\mathbf{r}_i) = U_{el} + U_b + U_m + U_C + e\phi(\mathbf{r}_i),
\]

where \( U_{el} \), \( U_b \), \( U_m \), and \( U_C \) are the electrostatic, the short-range Lennard-Jones interaction, the membrane interaction, and the Coulomb interaction energy, respectively, and \( e \phi(\mathbf{r}_i) \) is the external electrostatic potential due to the charges in the membrane and electrolyte. Note that there is no potential energy in equation (5) associated with bending of the polymer, i.e., the beads are freely linked together, because the persistence length of the ssDNA is found to be about the length of one nucleotide at high solution concentrations [40].

The energy associated with elastic bond stretching is described by a simple harmonic potential

\[
U_{el} = k_{el} \sum_{j=\pm 1} (r_{ij} - r_0)^2,
\]

where the spring constant \( k_{el} = 171 \text{ kcal mol}^{-1} \text{ Å}^{-1} \), the elastic equilibrium bond length \( r_0 = 2.5 \text{ Å} \), and \( r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| \) is the bond length between two \( i \)th and \( j \)th beads [39].

The short-range potential energy of the \( i \)th bead due to other beads (excluded volume effects) is modeled via the Lennard-Jones potential

\[
U_b = \epsilon_b \sum_{j \neq i} \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - 2 \left( \frac{\sigma}{r_{ij}} \right)^6 \right],
\]

where the interaction strength \( \epsilon_b = 0.1 \text{ kcal mol}^{-1} \) and \( \sigma = 6.5 \text{ Å} \) [39].

To describe the polymer–membrane interaction, we use a continuum Lennard-Jones potential instead of representing the membrane by a collection of Lennard-Jones atoms [41, 42] which in our case would be computationally expensive in view of the relatively thick membrane (25 nm). As such, in \( U_m \) we replace \( r_{ij} \) by the distance between the \( i \)th bead and the nearest point on the membrane surface and take \( \sigma = 2.5 \text{ Å} \) which is smaller than the value in \( U_b \) as beads can be closer to the membrane surface than to each other. For the chemically modified surface, it may be necessary to sample a region of the membrane surface to properly describe interaction between the biomolecule and the surface; this procedure can be easily incorporated in our model, albeit at the increased computational cost.

The screened Coulomb potential energy \( U_C \)

\[
U_C = \frac{e^2}{4\pi \epsilon} \sum_{j \neq i} r_{ij}^{-1} e^{-r_{ij}/2D},
\]

arises mostly from the presence of fixed phosphate backbone charges \( -e \) (contributions from small positive charges on bases and sugars are neglected) screened by the ionic charges in the solution.

Note that \( U_C \) does not account for the electrostatic interaction between the beads and charges in the membrane and on its surface. This effect is captured by the last term in equation (5) in which the electrostatic potential \( \phi(\mathbf{r}_i) \) is calculated from equations (1)–(3). Thus, the interaction of the polymer with the membrane has two contributions: (1) the short ranged Lennard-Jones interaction energy \( U_m \) which is due to the atomic structure of the membrane, and (2) the long-range Coulomb potential \( \phi(\mathbf{r}_i) \) arising in particular due to the presence of the static surface charge as well as the bulk dopant charges (both fixed and mobile, see equation (2)) and the external biases \( V_n \) and \( V_p \), see figure 1), with the last two being unique to our layered semiconductor membrane.

3. Results and discussion

The electrostatic potential in our layered membrane exhibits sharp variation around the center of the membrane due to the presence of the p–n–junction and high doping of layers, even in the absence of the applied biases, i.e., when \( (V_n, V_p) = (0, 0) \text{ V} \). Due to the presence of the depletion layer around the membrane surface preventing screening of this potential, the potential variation is carried over inside the nanopore provided the pore is narrow. Application of non-zero layer biases allows further tuning of the potential in a broad range [33] to either achieve its maximum possible variation for a given membrane–electrolyte system or mimic a neutral nanopore with a flat potential along the channel when needed.
cross-section. Even larger potential variations along and across the pore’s bulk electrolyte concentration, etc it is possible to produce nanopore geometry, dopant density, surface charge density, (figure 1(C))). By adjusting structure parameters such as $\sim$ flattest possible (deviations from the average value are within $|x| < 6$ Å) while the potential decreases (increases) away from the pore’s center towards the membrane surface (by $\sim 100$ mV) in the p(n)-layer where the electric field changes its direction and is oriented oppositely to the driving electric field from the electrolyte bias. The electrostatic potential decreasing towards the membrane’s surface in the p-layer means that the negatively charged ssDNA molecule will be somewhat attracted to the surface while different direction of the electric field $-\partial \phi / \partial z$ around $z \sim 125$ Å indicates that its translocation through the central constriction will also be inhibited.

In order to understand the biomolecule translocation dynamics in detail, we first consider the effect of the p–n-membrane potential on the evolution of the ssDNA and in particular its gyration radius $R_g = [((2N)^{-1}\sum_{ij} \xi_i^2 \xi_j^2)^{1/2}$ as the biomolecule permeates through a nanopore. One can see in figure 2(A) that while in the pore, the polymer’s gyration radius increases, i.e., the polymer extends, with respect to its equilibrium value of $R_g^{eq} \sim 12$ Å. For the flat p–n-potential (blue curve in figure 2), the maximum value of the gyration radius here ($\approx 23$ Å) is much smaller than $R_g^{eq}$ in the one-dimensional limit when all DNA beads are extended along a line.

To study the effect of a tunable p–n-junction potential on the ssDNA translocation dynamics, in this work we consider two membrane bias configurations: $(V_n, V_p) = (1.0, -1.0)$ V and $(-0.2, 1.2)$ V. In the absence of the electrolyte bias, the former produces the largest variation of the potential around the center of the pore ($\sim 50$ mV, see bottom inset of figure 1(C)), in the range of the membrane layer biases $|V_{nip}| \leq 1.2$ V, while the latter one corresponds to the flattest possible (deviations from the average value are within $\sim 5$ mV induced electrostatic potential in the nanopore (figure 1(C))). By adjusting structure parameters such as nanopore geometry, dopant density, surface charge density, bulk electrolyte concentration, etc it is possible to produce even larger potential variations along and across the pore’s cross-section.

When electrolyte bias is applied, the electrostatic potential computed from the solution of PNP equations for different membrane voltages, exhibits marked variations along the nanopore’s axis and cross-section. For $(V_n, V_p) = (-0.2, 1.2)$ V, $\phi$ drops almost linearly in the $z$-direction and remains virtually constant in the perpendicular radial direction. For $(V_n, V_p) = (1.0, -1.0)$ V however, the potential changes are more pronounced: it is much flatter (smaller driving electric field) around the pore’s center ($z \sim L/2$ Å and $|x| < 6$ Å) while the potential decreases (increases) away from the pore’s center towards membrane surface (by $\sim 100$ mV) in the p(n)-layer where the electric field changes its direction and is oriented oppositely to the driving electric field from the electrolyte bias. The electrostatic potential decreasing towards the membrane’s surface in the p-layer means that the negatively charged ssDNA molecule will be somewhat attracted to the surface while different direction of the electric field $-\partial \phi / \partial z$ around $z \sim 125$ Å indicates that its translocation through the central constriction will also be inhibited.

![Figure 2.](image-url) (A) Time dependencies of the gyration radius $R_g$ for $(V_n, V_p) = (1.0, -1.0)$ V (red) and $(V_n, V_p) = (-0.2, 1.2)$ V (blue). The arrows mark the times $t_{\text{in}}$ and $t_{\text{out}}$ when the center of mass of the molecule enters the pore and passes its center, respectively. $t_{\text{out}} = 362(214)$ μs is the time when the center of mass reaches the pore. (Complete videos of the translocation processes are available at stacks.iop.org/Nano23/255501/mmedia.) (B) Snapshots of the DNA configuration at specific times during translocation (shown by the black dots in (A)) for $(V_n, V_p) = (1.0, -1.0)$ V.

The extension of the biomolecule can be increased in a biased p–n-membrane where the local electric field around the center of the pore (see figure 1(C)) is oriented oppositely to the driving electric field from the applied electrolyte bias. This field holds the charged polymer molecule just above the nanopore’s constriction. This regime of the polymer translocation dynamics is manifested by a small value of $R_g \sim 14$ Å in the middle part of the curve for $(V_n, V_p) = (1.0, -1.0)$ V in figure 2(A). However, the specific p–n-electric field is not strong enough to hold the ssDNA molecule indefinitely, and, after some time, a configuration is realized that allows for polymer penetration of the potential barrier and subsequent polymer translocation towards the nanopore’s exit. During this process, the polymer again elongates $(R_g$ increases) while its ‘tail’ located above the constriction is still held by the strong membrane electric field (figure 2(B)), so that the polymer’s extension is significantly larger $(R_g \sim 35$ Å) than for the weak p–n-potential when only the geometric constriction of the molecule by the nanopore is present. Note that for a fixed p–n-potential (fixed $V_n$ and $V_p$), the reduction of $V$ leads to a smaller driving electric field so that a time during which a charged polymer remains trapped in the nanopore can in principle be varied.

As the electrostatic potential is not constant across the pore but is rather decreasing (increasing) away from the pore axis in the n (p) side of the membrane (figure 1(B)), the arising lateral electric field will have an additional straightening effect on the polymer on the n-side while alleviating biomolecule
entrance in the nanopore on the p-side by effectively lowering the potential barrier at the opening \([44]\). This additional focusing effect of the membrane potential is unique to our system. In fact, this asymmetry makes our p–n-nanopore somewhat similar to the α-HL biochannel with its wide vestibule and narrow β-barrel, with the added advantage that the electrostatic landscape across the membrane can be easily controlled and fine-tuned by the applied biases.

As the biomolecule motion is stochastic, we need to perform statistical analysis of the translocation results based on many (~3 × 10³) for each studied case) translocation events. For each event, we first relaxed the DNA for 0.1 ms in the absence of both pore and driving potentials, and then placed the relaxed polymer at a distance of \(2R_g^\text{eq}\) from the mouth of the pore and let the applied electrolyte bias capture it and drag it inside. We also record the DNA translocation time \(\tau = t_{\text{out}} - t_{\text{in}}\) as the difference between the times when the DNA’s center of mass enters the pore, \(t_{\text{in}}\), and when it emerges out of it, \(t_{\text{out}}\). Note that this way of defining \(\tau\) is only appropriate if the characteristic polymer size is much smaller than the membrane thickness, which is indeed the present case: the average length of the biomolecule in the nanopore is \(\sim 80\,\text{Å}\) which is much smaller than \(L\).

The resulting histograms for the translocation times \(\tau\) and respective average gyration radii \(\langle R_g \rangle\) are presented in figure 3. Due to the interaction of the ssDNA with the nanopore which allows the biomolecule to relax \([43]\) during its translocation, there is some spread in both \(\tau\) and \(\langle R_g \rangle\) values. When a p–n-electric field is present in the pore, the time during which the polymer remains localized around the center of the pore (small \(R_g\), see figure 2) depends on the ratio of the membrane potential drop in the pore to the ambient system temperature \([44]\): the larger the ratio, the smaller the probability to realize a biomolecule configuration which would allow penetration of the potential barrier. Thus, this time significantly varies from simulation to simulation, leading to a large spread in values of \(\tau\) and a much wider histogram \(P(\tau)\) in figure 3(A) with a long tail at large \(\tau\) for \((V_n, V_p) = (1.0, -1.0) \, \text{V}\). The average value of the translocation time in this case is larger as well (due to the induced delay in the polymer translocation), as expected.

Interestingly, while \(P(\tau)\) broadens with increasing membrane electric field in the pore, the histogram of \(\langle R_g \rangle\) narrows down (figure 3(B)). This is because of the long time during which the biomolecule is localized in the center of the pore, see figure 2, which increases the contribution of small \(R_g\) to the average gyration radius value, thereby decreasing \(\langle R_g \rangle\). However, \(R_g\) averaged only over the time when the molecule is within the n-layer (\(\langle R_g^{\text{eq}} \rangle\), green histograms with thin bars in figure 3(B)) is significantly larger for a strong p–n-junction electric field than for a weak one, consistent with the above discussion on the focusing effect of the p–n-junction potential on the biomolecule. Also, for the strong membrane field, we see that the biomolecule is always strongly extended (the histograms of \(\langle R_g^{\text{eq}} \rangle\) and \(\langle R_g \rangle\) are separated), while for the flat p–n-potential, the molecule is more coiled in the n-layer (the histograms of \(\langle R_g^{\text{eq}} \rangle\) and \(\langle R_g \rangle\) overlap) due to the relaxation after passing the nanopore constriction accompanied by gradual decrease in its length.

![Figure 3](image)

Figure 3. (A) Histograms of the translocation times \(P(\tau)\) for \((V_n, V_p) = (-0.2, 1.2) \, \text{V}\) (blue, left) and \((1.0, -1.0) \, \text{V}\) (red, right). (B) Histograms of the average gyration radii for the same membrane bias configurations \((V_n, V_p)\). The blue and red (thick bars) histograms are for \(\langle R_g \rangle = \tau^{-1} \int_{t_{\text{in}}}^{t_{\text{out}}} R_g(t) \, \text{d}t\) while the green ones (thin bars) are for \(\langle R_g^{\text{eq}} \rangle = \tau^{-1} \int_{t_{\text{mid}}}^{t_{\text{out}}} R_g(t) \, \text{d}t\). The dashed line corresponds to the equilibrium value of the gyration radius \(R_g^{\text{eq}}\).

Note that the average translocation time \(\langle \tau \rangle \sim 180 \, \text{µs}\) for the flat potential \((V_n, V_p) = (-0.2, 1.2) \, \text{V}\) is in agreement with the result of a simple drift model where the viscosity friction force \(\xi(L/\tau)\) is balanced out by the driving force of the applied electric field \(e(V/L): \tau = \xi L^2/(eV)\). We can also estimate the average ssDNA speed for this bias configuration as \(L/\tau \approx 1.5 \, \text{Å} \, \text{µs}^{-1}\) or ~0.5 nucleotides \(\text{µs}^{-1}\). This is consistent with results of experiments on DNA translocation \([26]\) and other calculations \([39]\) for an applied bias of \(\sim 0.1 \, \text{V}\).

4. Conclusion

In this work, by utilizing the PNP model of the membrane-electrolyte system together with Brownian dynamics simulations of the biomolecule, we show that ssDNA translocation through the double-conical nanopore formed in a semiconductor membrane consisting of p- and n-doped layers of Si is strongly affected by the presence of biased
p–n-junction potential. When there is a large electrostatic potential variation along the pore, the strong electric field localized around the pore’s center and oriented along the channel hinders DNA molecule translocation allowing us in principle to completely halt its passage if necessary; the value of the potential variation can be effectively controlled with the applied layer biases ($V_n$, $V_p$). In addition to this, the lateral electric field on the n-side of the pore produces an additional focusing effect on the DNA motion so that the polymer is unraveled and stretched far more than a simple geometric confinement of the neutral nanopore would allow. Such asymmetry between the biomolecule dynamics on the n- and p-sides of the nanopore channel makes our system a solid-state analog of the biological α-HL channel. It is also possible to envision other membrane structures where, for example, layers of graphene are sandwiched between p- and n-layers of doped semiconductor, thus allowing even more precise and robust control over the biomolecular dynamics.

The effect of slowing down and stretching the biomolecule can be further enhanced in structures with larger potential variations along the pore’s axis, which can be achieved in smaller pores or for smaller (larger) electrolyte (dopant) concentrations. However, these systems will likely require modeling via a particle approach such as BD simulations for both electrolyte and polymer. In general, the ability to control a polymer’s translocation process in a nanopore created in a p–n-membrane could be very beneficial for understanding the dynamics of biomolecules in nanopores and potentially, even for DNA sequencing.

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References

[14] Li J, Gershov M, Stein D, Brandin E and Golovchenko J 2003 Nature Mater. 2 611
[16] Storm A, Chen J, Ling X, Zandbergen H and Dekker C 2008 Nature Mater. 2 537
[27] Deamer D and Branton D 2002 Acc. Chem. Res. 35 817
[33] Nikolaev A and Gracheva M 2011 Nanotechnology. 22 165202
[34] Kong C Y and Muthukumar M 2002 Electrophoresis 23 2697
[37] Chung S H and Corry B 2005 Soft Matter 1 417
[40] Smith S B, Cui Y J and Bustamante C 1996 Science 271 795