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# Computational modeling of a rotary nanopump

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ABSTRACT

The dynamics of a rotary nanopump, consisting of three coaxial carbon nanotubes and a number of graphene blades, has been simulated via application of the molecular dynamics (MD) method. In this nanopump the inner nanotube, the middle carbon nanotube with together the graphene blades and the outer nanotube are used as the shaft, rotor, and sleeve of the pump, respectively. The rotary motion of the rotor is due to the mechanical rotation of the two first carbon rings of the rotor's carbon nanotube. We found that this pump flow the gas atoms between two sides of the nanopump and it can produce an atomic gradient. Also it is observed that a rotary frequency of the rotor affected on the pump performance for generating the density gradient and the maximum performance is occurred at a special frequency of the rotor. This special rotary frequency can be computed by an analytical formula, for given material and temperatures. Moreover, the results indicate that the number of the rotor's graphene blades do not have a significant effect on the pumping capacity. Our finding provides a potentially useful mechanism for gas purification process.



## 1. Introduction

The protein motors, which generate mechanical motion from chemical energy, play an important role in all life processes. These nanomotors can be divided into two main groups. The first group is the rotary nanomotor such as $F_0F_1$-ATP synthase [1,2] or bacterial flagella protein motor [3] that produces the rotary motion from the stored energy in the ion gradient between two sides of the motor. The second group is the linear motor such as myosin and kinesin [4] protein motors. These linear motors transport a variety of cargoes, like vesicles, in the stochastically fluctuating intracellular medium by using the chemical energy, released during the hydrolysis of the ATP (adenosine three phosphate) molecules.

Inspired by the protein motors, nano-scale motors can be proposed to use in nanotechnology. The single-walled carbon nanotubes (SWCNTs) are usually used to design nano-scale devices, such as nanomotors [5–7], nanopump [8–10], nanocarrier [11], bearings [12] and oscillators [13]. Here, we briefly review some of the conceptual nanomotors that have been designed in the past. Tuzun et al. have developed a laser-driven nanomotor [5], which is simulated by application of the molecular dynamics (MD). This nanomotor is constructed of two concentric nanotubes, acting as a sleeve and a shaft, where a pair of positive and negative electric charges was located on two carbon atoms of the end ring in the sleeve part. An oscillating electric field is used to induce a rotary motion in the sleeve. The full rotary motion is observed just at an optimum range of the field's frequency that the optimum range of the field's frequency is dependent on the size of the motor, and the relative positions of the attached charges.

Another MD simulation studied, Han et al. investigated the stability of the mechanically-driven nanogear [6]. They demonstrated that when the atoms near the end of the nanotube in one gear are enforced to rotate, the second nanotube begins to rotate as well.

In the other simulation [7], a nanoscale rotary motor driven by electron tunneling was examined. In this studied, the nanomotor is made of a carbon nanotube as a shaft with covalently attached isolating molecular stalks ending with conducting blades. Periodic charging and discharging of the blades at two metallic electrodes maintains an electric dipole on the blades that was rotated by an external electric field.

A further MD-based simulation has designed a nanopump [10] by using single-walled carbon nanotube (SWNT) to pumping molecules along the SWNT axis, via mechanical wave propagation driven by an oscillating tip actuator.

Recently, another MD-based simulation studied [14], a nanopropeller formed from a functionalised (8,0) SWCNT. The propeller pumped liquid due to an imposed rotation on its blades. The blades were made from pyrene molecules and attached to the opposite

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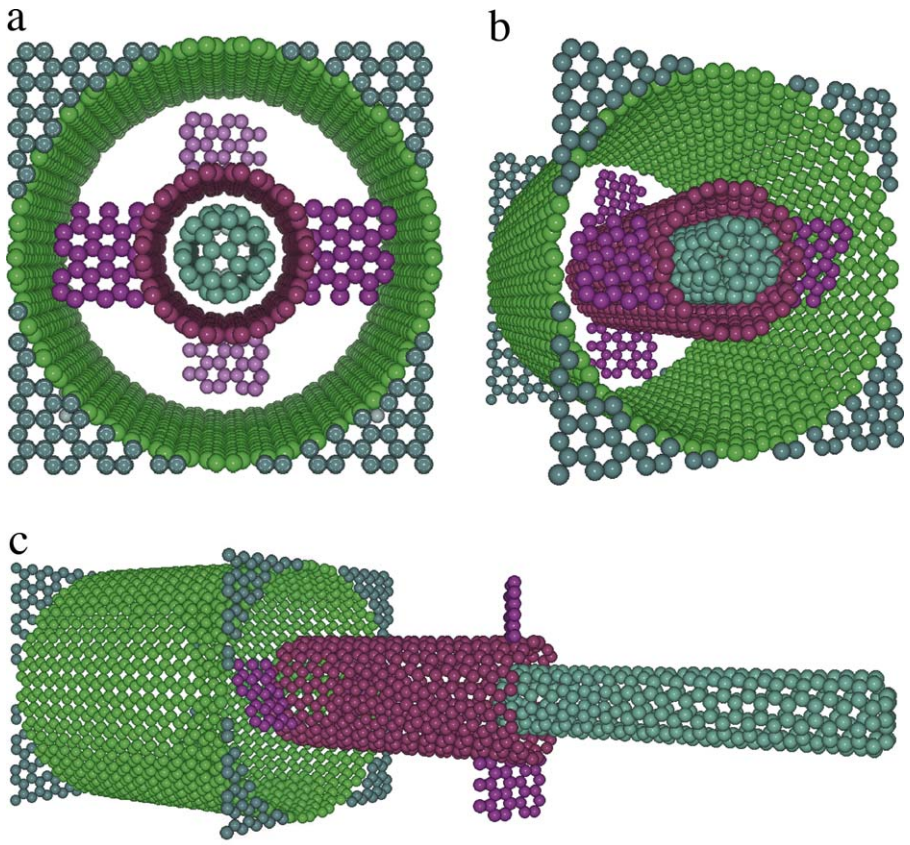


**Fig. 1.** The structure of the nanopump components: (a) front view of the rotor. The rotor is composed of a nanotube and four graphene blades attached to the opposite sides of the rotor at distal ends of the rotor axis and tilted with respect to its axis; (b) three dimensional view of of the nanopump; (c) the complete structure of the nanopump that shown separately.

sides of the nanotube and were tilted with respect to its axis. The simulation revealed that pumping depended significantly on the chemistry of the blade–liquid interface and also to the size, shape, chemical, or biological compositions of the nanoblades.

In our previous work [15], we proposed a nano-scale ion-driven rotary motor inspired by the $F_0$ part of ATPase protein-motor. That motor was constructed from SWCNTs, benzene rings and graphene sheets. The dynamics of that nanomotor in the presence and absence, of an external electric field has been simulated via stochastic molecular dynamics. The rotary motion of the proposed motor was resulted from an ion gradient established between the outer and inner parts of the environment containing the motor.

In this paper, we have proposed a nano-scale pump constructed of SWCNTs and graphene blades. The classical MD simulation [16] has been employed to simulate the dynamics of this rotary nanopump.

## 2. Atomistic structure of the proposed nanopump

The schematic structure of the proposed nanopump is shown in Fig. 1. Our proposed nanopump is composed of three sections. The first section is the shaft, which is made of a (5,5) capped nanotube with a length of 40 Å and a radius of 3.443 Å. The second section of the nanopump, named *rotor*, is made of a (10,10) nanotube with the same shaft length and a radius of 6.9 Å. As shown in Fig. 1(a) and (c), two pairs of graphene blades with the same area equal to $8.4 \times 6$ Å$^2$, are attached to the two ends of the rotor and tilted with respect to the rotor's axis. The third section of the nanopump is made of a (25,25) nanotube with a radius of 17.33 Å and is named the *pump sleeve*, which surrounds the rotor. Two identical boxes connect to the sides of the pump, one initially empty and the other filled with gas atoms. Since the boxes are cubic and the pump is cylindrical, two square graphene sheets are added to the pump to force the gas atoms to pass only through the pump to travel between boxes. These square graphene sheets have a central hole with a radius of 18.7 Å and are attached to the two ends of the pump sleeve.

## 3. Computational details

Our system has 1250 gas atoms. The number of carbon atoms in the nanopump is 2967, 3021 and 3075 for the rotor with two, four and six blades, respectively. The particles are confined in a rectangular box with dimensions of $L_x = 300$, $L_y = 37$ and $L_z = 37$ Å. Periodic boundary conditions are applied in the $y$- and $z$-directions and the temperatures is varied between 50 and 1100 K.

Two types of interatomic potential are used in our simulations. The first generation of Brenner potential [17] is used for modeling the covalent bonding between the carbon (C) atoms within the nanotubes and within the graphene blades. The Lennard–Jones (LJ) potential is used to describe the non-bonding interactions between the gas atoms and the carbon atoms as well as for carbon–carbon interactions between the different parts of the nanopump. The parameters of the LJ potential are $\epsilon_{Ne} = 0.003121$ eV, $\sigma_{Ne} = 2.75$ Å or $\epsilon_{He} = 0.000867$ eV, and $\sigma_{He} = 2.55$ Å [18], for the gas atoms, and $\epsilon_C = 0.002413$ eV and $\sigma_C = 3.4$ Å for the C–C interaction [18]. The parameters for the gas atoms and carbon atoms interaction are calculated by using the Lorentz–Berthelot mixing rules, i.e., $\epsilon_{\text{gas}-C} = \sqrt{\epsilon_{\text{gas}} \times \epsilon_C}$, and $\sigma_{\text{gas}-C} = 0.5(\sigma_{\text{gas}} + \sigma_C)$.

The dynamics of all atoms are described by Newton's differential equation and velocity Verlet method [16] is used for time integration, with a time-step of 0.5 fs. The simulations are