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Intrinsic edge warping of graphene nanoribbon boost molecular directional motion: Toward the novel nanodevices

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ABSTRACT

In this letter, nanodirectional motion due to intrinsic warping edge of graphene nanoribbon is demonstrated using theoretical analysis and molecular dynamics (MD) simulation. Simulation model is established and the underlying physical insights of intrinsic nanodirectional motion are investigated. It is found that nanodirectional motion of carbon fullerene is gradient-dependent. Directional motion with $+z$-warping graphene edge is energetically favorable over the $-z$-warping configuration. As a result, a novel nanodirectional motion actuator inspired by intrinsic edge warping with Gaussian curvature can be designed. The obtained results in current research are fundamental and general, similar intrinsic properties and design paradigms can be applied to other 2D materials beyond graphene.

Since the famous apple fell on Isaac Newton, mankind seemed finally in a position to under the rules of the game that gravity played. From then onwards, utilizing intrinsic mechanism like gravity that leads to machinery with directional motion presents a promising approach for the scientific research community. Especially, the bottom-up perspective gives us an inspiration in speed-up of the search with respect to directional transport mechanism.

Renormalization of physical properties at nanoscales offers the scalability of exquisite separability in the delivery of mass. However, extending directional motions at nanoscales to a facile machinery may require mapping the fundamental building blocks to a desired target model, which the external excitations [1–3] undoubtedly raise the difficulties. Therefore, we advocate aiming at developing intrinsic interactions [4–6] to response such a problem.

As an intrinsic nature, edge warping is most frequently ascertained in atomically thin materials especially the graphene [7,8], which edge effects serve as a crucial ingredient in changing their properties in relation to mechanics and condensed matter physics [9–11]. However, there is still no well documented on intrinsic edge warping as a driving force to boost nanodirectional motions, which may impose restrictions on the scalability of design space in terms of nanodevices. To address this issue, we demonstrate the fundamental directional motion by designing a simple nanomechanical system comprised of a graphene substrate and a carbon fullerene (C_{60}). The essence of our design paradigm is that after forming intrinsic warping of graphene substrate in pairs we have a surface with built-in curvature gradient, with the delicate variation in distribution of van der Waals (vdW) interaction, the resultant net force can cause the carbon fullerene to move directly. While our model is carried out to unveil the feasibility of directional motion induced by intrinsic edge effect, the similar design paradigm or topological reconfiguration buildup can be applied to design novel nanodevices such as curvature-driven motion converters, energy actuators or nanowindings of incising the magnetic line.

For an atom $(L/2, 0, A+h)$ positioned above a warped graphene with a free edge as detailed in Fig. 1(a) (A is the warping amplitude of graphene substrate, h is the equilibrium distance between the atom and graphene), y-directional motion of the specific atom is responsible for midline carbon atoms $(L/2, y, z)$ due to the symmetry of warped graphene. To establish a framework of continuum cohesive model, the carbon atoms in the graphene are homogenized by surface density ρ_c, which represents the number of carbon atoms per unit area, and is dependent on the carbon–carbon bond length l_0 by $\rho_c = 4/(3\sqrt{3}l_0^2) \approx 40\ \mathrm{nm}^{-2}$. It is important to note that the surface density may be slightly different from the flat graphene. The energy between two atoms with a distance r due to van der Waals force is usually represented by Lennard-Jones 6–12 potential, $V(r) = 4\varepsilon(\sigma^{12}/r^{12} - \sigma^6/r^6)$, where $\sqrt[6]{2}\sigma = h$ and ε are distance and bond energy between atoms in equilibrium state, respectively. Moreover, the

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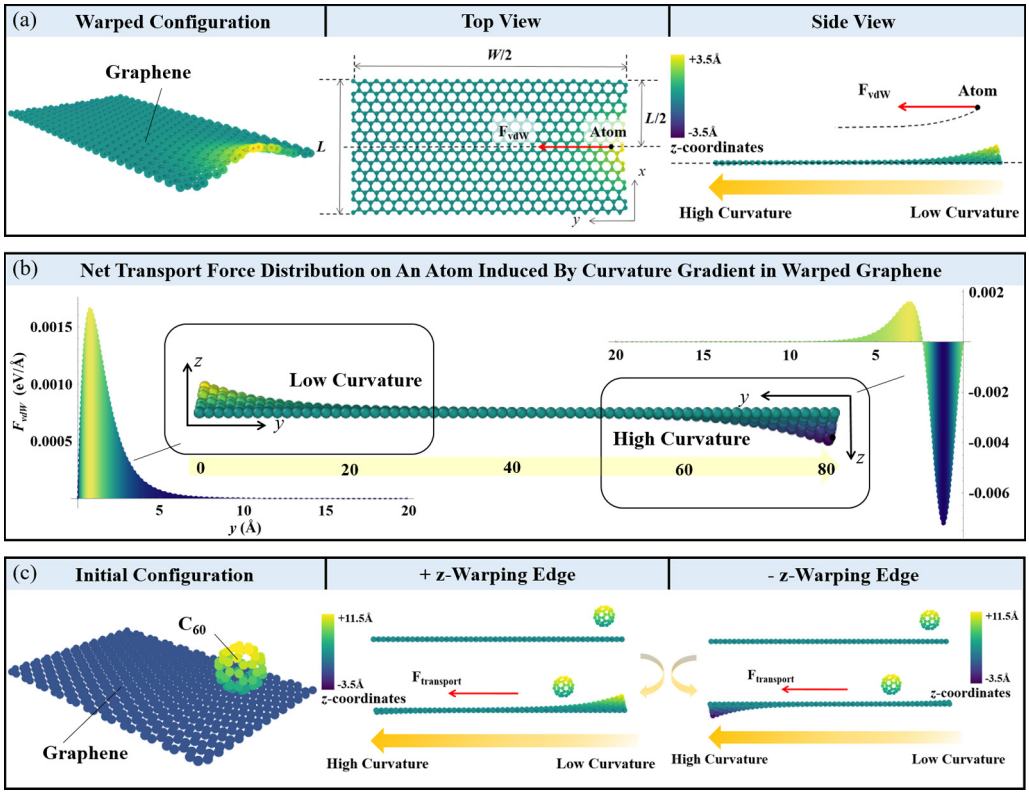

Fig. 1. (a) Schematic of an analytical model for an atom above a warped graphene with $+z$-warping free edge. (b) Net transport force distribution of an atom induced by curvature gradient in warped graphene. (c) Illustration of two typical models with C_{60} and an isolated free edge. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

warping configuration of graphene nanoribbon can be described by surface function $z(x, y) = A\sin(\pi x/L)e^{-y/c}$, where L and c are the length and penetration depth of graphene nanoribbon, respectively, A is the warping amplitude. The distance between the specific atom and the midline carbon atoms can be calculated by $r = \sqrt{y^2 + (Ae^{-y/c} - A - h)^2}$. By utilizing the lattice symmetry of graphene substrate, the midline cohesive energy between the atom and the warped graphene can be given by $\psi_{line} = \rho_c \int_{ls} V(\sqrt{y^2 + (Ae^{-y/c} - A - h)^2})ds$. The net force acting on the specific atom because of warped graphene can be evaluated analytically to give $F_{vdW} = -d\psi_{line}/dy > 0$, that is, built-in curvature gradient of intrinsic edge for graphene nanoribbon can lead to the net transport force and nanodirectional motion.

For specific graphene nanoribbon ($c = 7.3$ Å) with $L = 30$ Å and $W/2 = 40$ Å, Fig. 1(b) plots the F_{vdW} of a specific atom as a function of y-direction location based on above theoretical derivation. Two important observations should be reported: typical evolution for net transport force F_{vdW} is nonlinear: first a linear increase followed by a drop at somewhere from $y = 2$ Å to $y = 5$ Å, after which the net transport force varies in a much lesser extent (≈ 0 eV/Å). Moreover, nanodirectional motion is curvature-oriented: the specific atom will move from low curvature to high curvature for warped graphene. To verify our speculation, the molecular dynamics (MD) simulation is performed using the LAMMPS simulation package [12], in which the adaptive intermolecular reactive empirical bond order (AIREBO) potential [13] is utilized to model the C–C atoms interactions (cutoff distance of REBO is assigned to be 2 Å [14]). As a demonstration, we investigate the directional motion of carbon fullerene as indicated in Fig. 1(c), the interlayer interaction of C_{60} and graphene is described by LJ potential ($\varepsilon = 2.968$ meV and $\sigma = 0.3407$ nm). All MD simulations are performed using the microcanonical ensemble and Berendsen thermostat at 0.1 K with the time step of 0.001 ps.

Free edges normally show up in pairs, Fig. 1(c) illustrates two typical configurations for isolated free edge after initial equilibrium, i.e. $-z$ warping configuration (high curvature) and $+z$ warping configuration (low curvature). Using MD simulation we find that intrinsic edge warping of graphene nanoribbon can construct a curvature gradient, and lead to a vdW potential gradient that drives the C_{60} to move towards high curvature. Importantly, the present finding demonstrates the intrinsic edge warping of graphene can boost the motion of the molecule.

Fig. 2(a) and Fig. 2(c) present several typical snapshots of nanodirectional motion where the C_{60} is moving along the $-z$-warping graphene and $+z$-warping graphene, respectively. Apparently, when $-z$-warping edge forms and generates a positive curvature, C_{60} slides towards the $-z$-warping edge and followed by a degraded oscillation at the end (see solid lines in Fig. 2(e) and Fig. 2(f)). It is important to note that the triggered distance between C_{60} and $-z$-warping edge is about 28 Å. The C_{60} will move towards the flat region for $+z$-warping-edge-formed negative curvature surface (see dash lines in Fig. 2(e) and Fig. 2(f)). Comparing Fig. 2(e) and Fig. 2(f) show that the $+z$-warping edge is energetically favorable over the corresponding $-z$-warping edge, and the highest velocity and acceleration of the C_{60} are respectively 0.66 Å/ps and 0.04 Å/ps^2. Moreover, the tendency of acceleration for $+z$ and $-z$-warping edge of graphene, in essence, is in line with the derivation. It is seen from Fig. 2(e) that z-directional edge warping of graphene can be effectively converted into y-directional motion of the C_{60}. To gain more physical insights into the intrinsic-edge-warping-driven mechanism, the atom potential energy of the C_{60} (Fig. 2(b) and Fig. 2(d)), the interlayer vdW potential energy and total potential energy of the system (Fig. 2(g)) are investigated using MD simulation. As shown in Fig. 2(b) and Fig. 2(d), the net force $F_{transport}$ of the C_{60} results from the potential distribution difference, large parts of high potential energy are on the left side

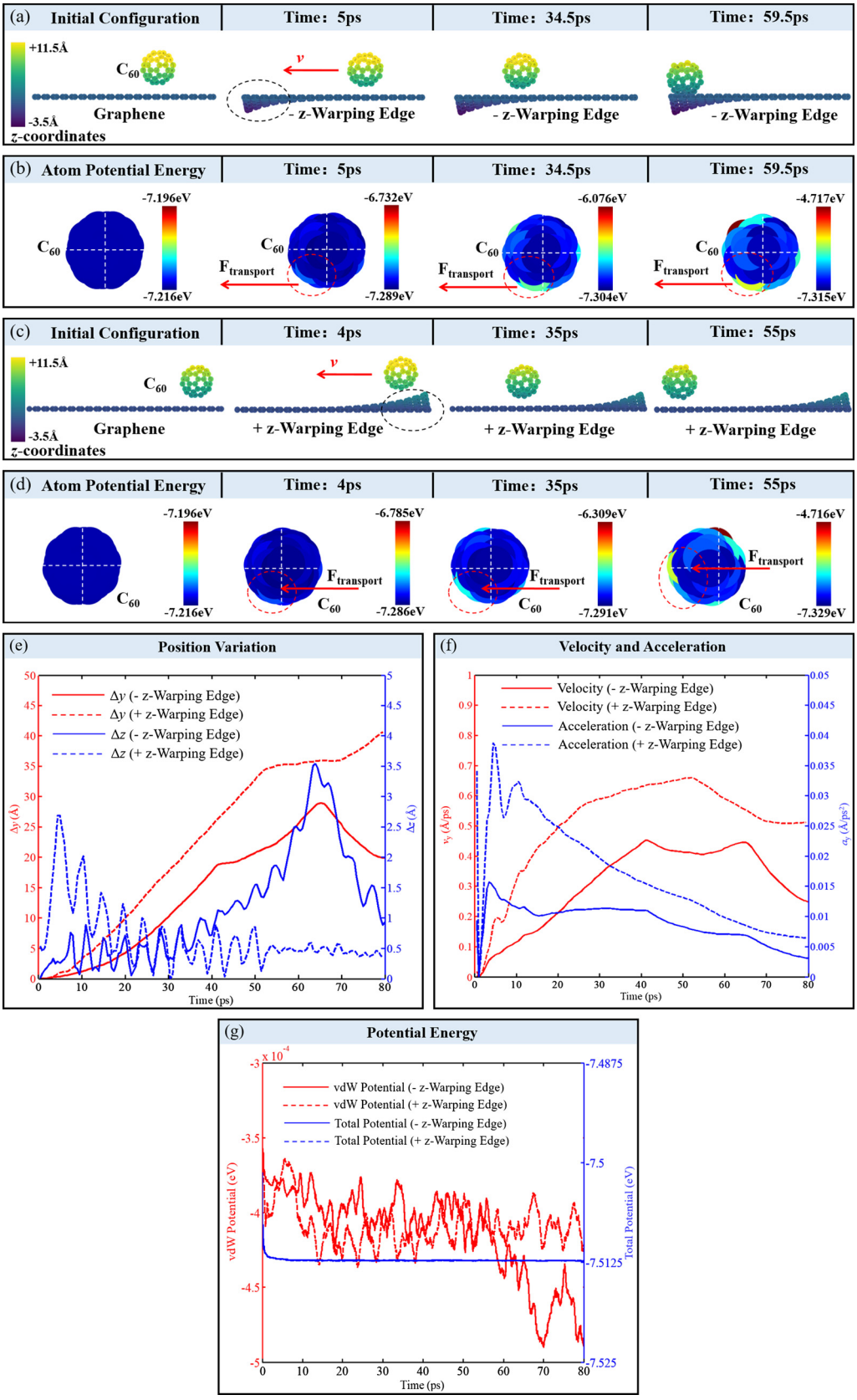

Fig. 2. Snapshots of nanodirectional motion for C_{60} with (a) $-z$-warping graphene edge and (c) $+z$-warping graphene edge. The corresponding atom potential distribution of C_{60} for (b) $-z$-warping edge and (d) $+z$-warping edge. (e) Position variation of C_{60} for nanodirectional motion with regard to Δy and Δz. (f) Velocity and acceleration variation of C_{60} for nanodirectional motion with regard to v_y and a_y. (g) The vdW potential energy and total potential energy versus the simulation time.

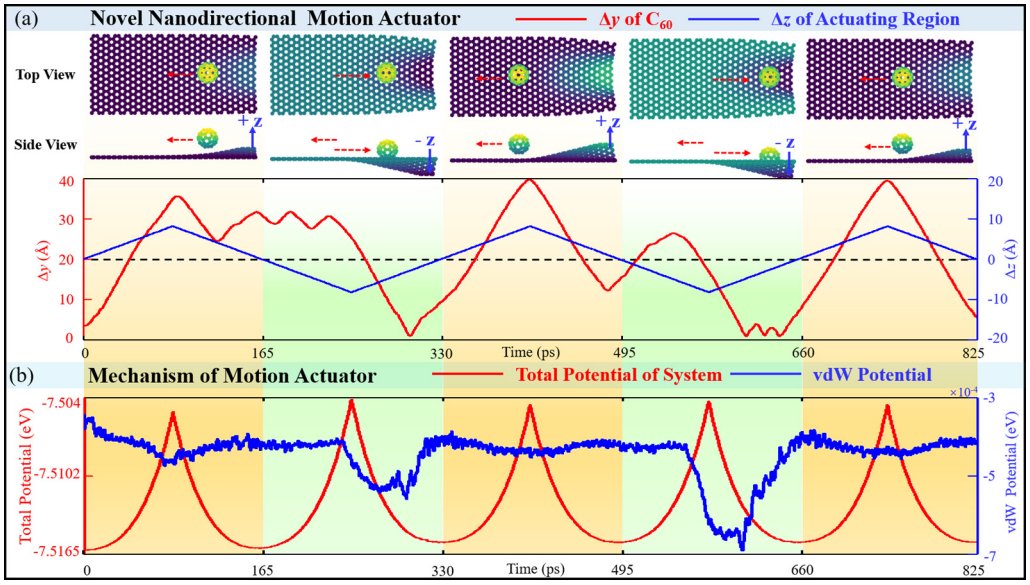

Fig. 3. Novel nanodirectional motion actuator based on "artificial edge warping" concept. (a) Δy of C_{60} and Δz of actuating region versus the simulation time using MD simulation. (b) vdW potential energy and total potential energy of the system versus the simulation time.

of C_{60} because of built-in curvature gradient of warping graphene. From an energy point of view, the bending energy of graphene E_{BG} and bonding energy E_{Bond} can be neglected in the current C_{60}/graphene system, as the configuration of warping graphene is stable and no rebonding/bond-breaking occurs during the MD simulation. Consequently, the net force $F_{transport}$ is attributed to the vdW potential energy E_{vdW} and deformation energy E_{Deform} of the C_{60}. Depending on the curvature increasing, the C_{60} shows a larger contact area with graphene, indicating higher E_{Deform} of the C_{60} molecule. As for E_{vdW}, reductions in energies result from the dilution effect of increasing carbon atoms density. Fig. 2(g) captures typically variation in E_{vdW} that extracts additional values calculated by the LJ potential. Clearly, total potential energy is almost unchanged. However, as the curvature (or time) is increased, the case of $-z$-warping edge has a more steep decreasing, which is highly warranted by increased E_{Deform}. It is important to note that, for C_{60} molecule with $-z$-warping edge, E_{Deform} provides a resistance.

From the viewpoint of mechanics, Fig. 2(g) indicates that $-z$-warping and $+z$-warping are two stable states with the same potential, that is, intrinsic edge warping of graphene is bistable. To switch such two configurations between each other, the potential barrier from warping to flat state of graphene should be overcame. Therefore, building systems with complex behavior from intrinsic natures, such as a novel nanodirectional motion actuator with C_{60} and graphene, may require an intermediary between the topology due to intrinsic property and the targeted functionality. Here, we first introduce the "thermal perturbation" method. We suppose the potential energy barrier is ΔE and the number of warping carbon atom is $N_{warping}$, clearly, the energy barrier per atom is about $\Delta E/N_{warping}$. Additionally, the probability to overcome ΔE is proportional to $e^{-\Delta V/k_B T}$. This implies that, using thermal effect the warping direction of graphene may be flipped, resulting motion transformation of C_{60} molecule due to curvature variation of graphene nanoribbon. Information on additional simulations and the relevant theory is available in Ref. [15].

However, the "thermal perturbation" method is probabilistic, another novel concept should be proposed. Inspired by topological surface with Gaussian curvature of intrinsic warping, as outlined above, we successfully design a nanodirectional motion actuator based on so-called "artificial edge warping" concept as shown in Fig. 3(a). Creating an actuating region in the free edge of graphene that leads to controllable Gaussian curvature presents a novel design paradigm. Molecular dynamics (MD) simulation is performed to investigate the nanodirectional reciprocating motion of the C_{60} molecule. Fig. 3(a) reveals that if the actuating region is reciprocally moving with 3.03 GHz, the oscillation amplitude of y-directional motion for C_{60} is significantly larger than that of z-directional motion for actuating region. This implies that the novel motion actuator we designed here has a great conversion efficiency for intrinsic-edge-warping-driven nanodirectional motion. As seen in Fig. 3(b), as the absolute value of the curvature is increased, the total potential energy increases and the E_{vdW} decreases. E_{vdW} provides a driving force for moving the C_{60}, which is in parallel to our theoretical demonstration. Equally, based on the above results we propose the idea of a nanochannel induced by intrinsic edge warping of graphene nanoribbon. The description of such an idea is shown in Fig. 2(b), which produces a larger nanodirectional distance. It is of interest to know how the results in this research for the whole graphene nanoribbon, the authors will answer this question in the near future.

In conclusion, this research has, through theoretical analysis and MD simulations, for the first time, revealed intrinsic edge warping of graphene nanoribbon can boost molecule (C_{60}) directional motion. Some remarkable conclusions are as follows.

(1) For an atom positioned above a warping graphene, the larger absolute value of curvature leads to the larger net transport force.
(2) Molecule and atom will move towards a higher curvature because of the resultant vdW potential gradient.
(3) Directional motion with $+z$-warping configuration is energetically favorable over the $-z$-warping configuration as the higher y-direction velocity and acceleration.
(4) Knowledge of intrinsic edge with Gaussian curvature can serve as a promising building block for constructing the novel nanodirectional motion actuator and be effective in speed-up of searching the intrinsic-nature-driven nanodevices.

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