Supplementary Information

Directional Control of Surface Rolling Molecules Exploiting Non-uniform Heat Induced Substrates

Alireza Nemati,[a] Hossein Nejat Pishkenari,[b] Ali Meghdari,[b] Shuzhi Sam Ge,[a,c]

[a] Institute for Future (IFF), Qingdao University, Qingdao 266071, China

[b] Center of Excellence in Design, Robotic and Automation (CEDRA), Sharif University of Technology, Tehran, Iran

[c] Department of Electrical and Computer Engineering, National University of Singapore, 119077, Singapore

Table of Contents

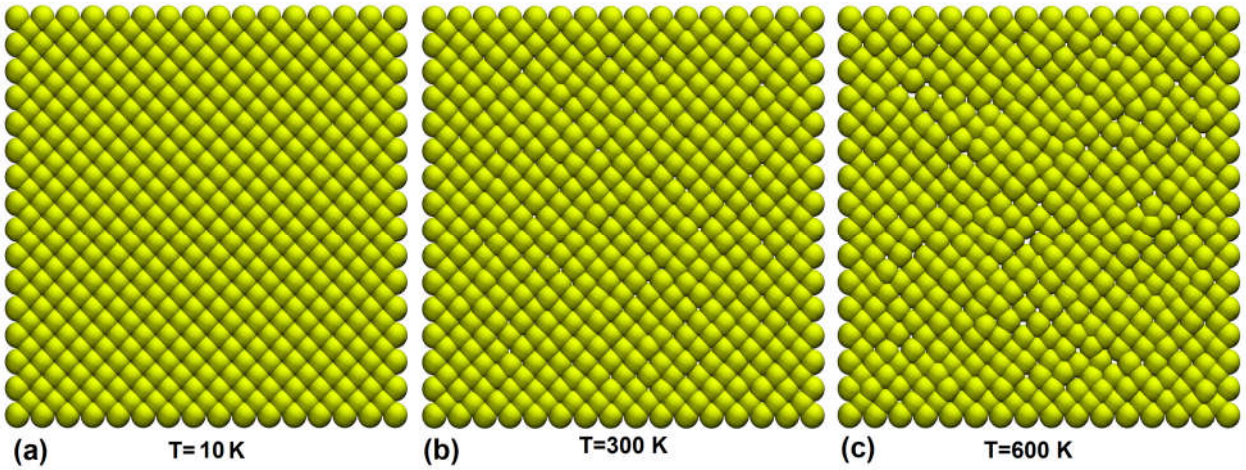

Figure S1. The structure of the top layer of gold atoms of the substrate at the temperature of a) 10 K, b) 300 K, and c) 600 K. The irregularity in the substrate structure result intensified fluctuation of the c60 binding energy during its movement on substrate.

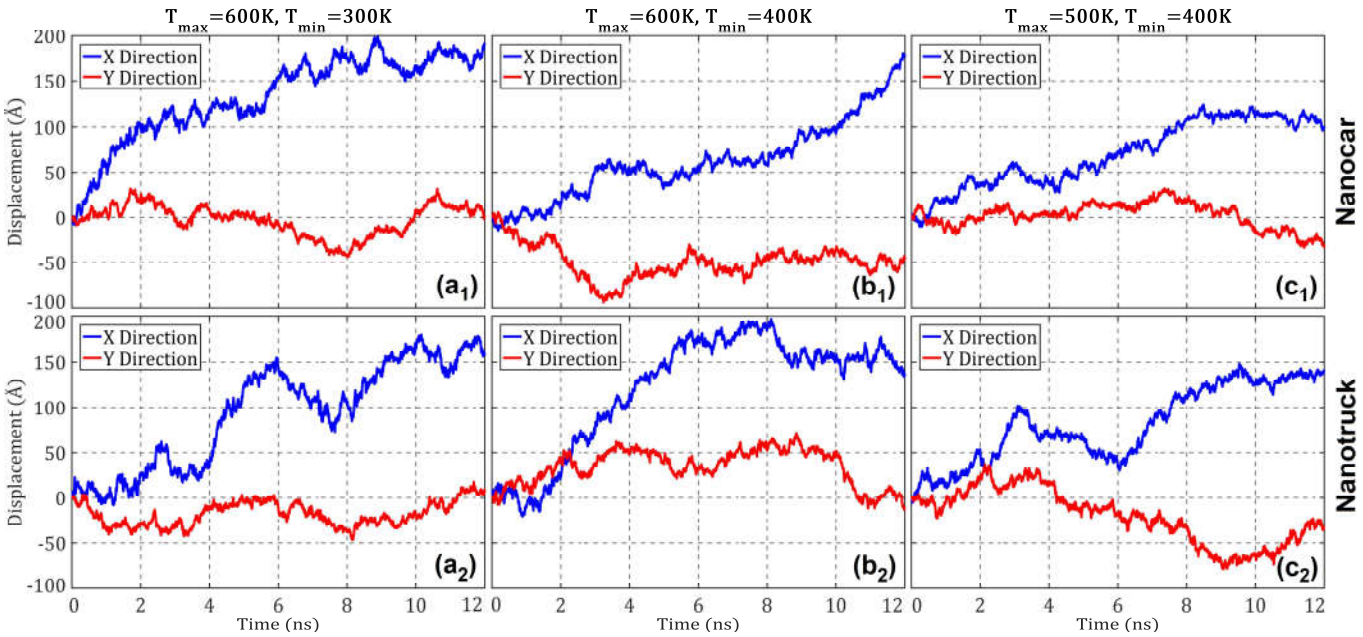

Figure S2. The displacement of nanocars along and perpendicular to the temperature gradient at different temperature distribution cases: a1) 600-300 K, b1) 600-400 K, c1) 500-400 K, a2) 600-300 K, b2) 600-400 K, and c2) 500-400 K. The results show that the motion of the studied molecular machine was affected by the temperature gradient since their motion along the X direction (along the gradient) is faster and has a longer range compared to their mobility in the Y direction (perpendicular to the gradient).

The 6-12 Lennard-Jones potential used in this study is presented in Equation 1. The ε shows the potential energy at the equilibrium distance, and σ is the distance at which the potential energy is zero.

$$E_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \qquad r < r_{cut-off} \tag{1}$$

Table S1. The Lennard-Jones parameters employed in this study

ε (eV)	σ (Å)	Description	ε (eV)	σ (Å)	Description
0.01273	2.994	C2-Au	0.01273	2.994	CA-Au
0.01315	2.611	H-Au	0.00190	3.460	CA-CA
0.01423	2.886	N-Au	0.00213	3.350	CA-N
0.00190	3.460	C2-C2	0.00197	3.647	CA-H
0.00230	3.244	N-N	0.00190	3.460	C2-CA
0.00204	2.673	H-H	0.00197	3.647	C2-H
0.00213	3.350	C2-N	0.00220	2.958	N-H

The form of the angle terms used in this study is presented in Equation 2, and the employed parameters are listed in Table S2.

$$E_{angle} = K_a(\theta - \theta_0)^2 \tag{2}$$

Table S2. The angle parameters used in the simulations

K_a $(\frac{eV}{rad^2})$	θ_0	Description
1.46619	π	C2-C2-CA
1.34141	2π/3	C2-CA-CA
1.34141	2π/3	CA-CA-CA
1.12304	2π/3	CA-CA-H
1.34141	2π/3	CA-CA-N
1.34141	0.638π	CA-N-CA

Equation 3 shows the bond terms employed in this study, and the related parameters are listed in Table S3.

$$E_{bond} = K_b(r - r_0)^2 \tag{3}$$

Table S3. The bond parameters used in the simulations

K_b $(\frac{eV}{Å^2})$	r_0 (Å)	Description
48.6652	1.212	C2-C2
30.8837	1.313	C2-CA
25.1593	1.392	CA-CA
14.35	1.101	CA-H
34.596	1.260	CA-N

The form of the dihedral terms employed in this study is presented in Equation 4, and its related parameters are listed in Table S4. The K_{d3} and K_{d4} parameters are zero due to the structure of the nanotruck and the nanocar.

$$E_{\text{dihedral}} = \frac{1}{2}K_{d1}(1 + cos\,\varphi\,) + \frac{1}{2}K_{d2}(1 - \cos 2\varphi) + \frac{1}{2}K_{d3}(1 + \cos 3\varphi) + \frac{1}{2}K_{d4}(1 - \cos 4\varphi) \quad (4)$$

Table S4. The angle parameters used in the simulations

$K_{d1}(eV)$	$K_{d2}(eV)$	Description
0	0.0000434	CA-C2-C2-CA
0	0.0000434	C2-C2-CA-CA
0	0.650451	C2-CA-CA-CA
0	0.650451	C2-CA-CA-H
-0.0403	0.208144	CA-CA-CA-CA
0	0.234379	CA-CA-CA-H
0.0433	0.650451	CA-CA-CA-N
0	0.390271	H-CA-CA-H
0	0.650451	H-CA-CA-N
0	0.433634	N-CA-CA-N