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Mechanical actuators at the nanoscale: molecular propellers, paddles and wheels LELA VUKOVIC, BOYANG WANG, PETR KRAL, University of Illinois at Chicago — We model by molecular dynamics simulations nanosystems that could realize mechanical action in nanofluidics. First, we study molecular propellers formed by carbon nanotube rotors with attached aromatic blades that can pump liquids with efficiency dependent on the chemistry of the liquid-blade interface [1]. Next, we investigate nanorods with photoactive surfaces that can roll on water when driven by light [2]. Their rolling motion is realized when chromophores attached to their surfaces become anisotropically polarized by light and attracted to water. Finally, we examine nanoscale pumping induced by deformable nanoscale blades [3]. We show that the length, polarity, frequency and amplitude of oscillations of the nanoblades control their efficiency of water pumping.

[1] B. Wang and P. Král, . Rev. Lett. 98, 266102 (2007).
[2] L. Vukovic and P. Král, submitted.
[3] L. Vukovic, D. Astumian and P. Král, in preparation.

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