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**Rotary molecular motion at the nanoscale: motors, propellers, wheels** LELA VUKOVIC, BOYANG WANG, PETR KRÁL, University of Illinois at Chicago — We describe by molecular dynamics simulations nanoscale systems that could realize rotary motion. First, we study molecular propellers formed by carbon nanotube rotors with attached aromatic blades [1]. We show that these propellers could pump different types of liquids, and their pumping efficiency strongly depends on the chemistry of the (hydrophobic or hydrophilic) liquid-blade interface. We also investigate nanoscopic wheels with hydrophobic surfaces that show rolling activity on water when driven. Finally, we model efficient molecular motors driven by electron tunneling, which could drive rotary molecular systems [2].

[1] B. Wang and P. Král, . Rev. Lett. 98, 266102 (2007).

[2] B. Wang, L. Vukovic and P. Král, Phys. Rev. Lett. 101, 186808 (2008).

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