One-way rotation of a molecule-rotor driven by a shot noise

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ELECTRONIC SUPPLEMENTARY INFORMATION

Figure S1. Asymmetric potential energy profile for a forced rotation of the molecule motor with one of the ferrocene-terminated arms truncated. Calculations were carried out with the semi-empirical ASED+ method.

Figure S2. Potential energy as a function of the torsion and rotational angle. The analytic form used here resembles the one given by equation (1), but differs from it by the introduction of an exponential factor, a Gaussian, whose purpose is to select one of the maxima shown in figure 4, making the others vanish. Its form is given by $V_0 \sin(\theta+\varphi)^2 \cos(\theta+\varphi)^2 e^{-\varphi^2} e^{-(\theta+\varphi)^2/s^2} + k\varphi^6$. The curves represented in color are the minimum energy paths (MEP) calculated with a custom-made nudged elastic band algorithm (NEB). The red curve is calculated starting form the right and going left, and the white one departs from the left and proceeds towards the right. Final and starting points of the two paths are fixed and coincide. However, the 12 intermediate points can move, their displacement being given by the force analytically derived form the potential, orthogonal to the path, and a spring force exerted on each point parallel to the path. The resulting force is subject to minimization, this was performed by a classic steepest descent method. After a number of iterations, the intermediate points have moved form their initial linear configuration and two different MEPs have been found that depend on the order of point calculation *i. e.* on the direction the path is followed.

Figure S3. Damping behaviour of the system model at different friction coefficient values. The black line represents an under-damped scenario, the blue line a critically damped scenario and the red line an over-damped scenario.