Nanoscopic friction under electrochemical control: supplementary material

POTENTIAL ENERGY FUNCTIONS

The potentials, $V^{\mathrm{t-d}}$ and $V^{\mathrm{d-d}}$, describing the tip-dipole and dipole dipole interactions respectively, can be written as a sum over positions of the tip atoms, $\mathbf{R}_j^{\mathrm{t}}$ (defined below), and the charges at the dipoles:

$$V^{\mathrm{t-d}} = \sum_{i=0}^{N-1} \sum_{j=0}^{n-1} V_i^{\mathrm{tip}}(X_j) \ , \tag{S1}$$

$$V^{\mathrm{d-d}} = \sum_{i} V_{\mathrm{dipole}}(\phi_i, \phi_{i+1}) \ , \tag{S2}$$

Here,

$$V_i^{\mathrm{tip}}(X) = \frac{qQ}{n} \sum_j [V_e(|\mathbf{R}_j^{\mathrm{t}} - \mathbf{r}_{i+}|) - V_e(|\mathbf{R}_j^{\mathrm{t}} - \mathbf{r}_{i-}|)] + \sum_j V_{\mathrm{c}}(|\mathbf{R}_j^{\mathrm{t}} - \mathbf{r}_{i+}|) \ , \tag{S3}$$

$$V_{\mathrm{dipole}}(\phi_i, \phi_j) = qq[V_e(|\mathbf{r}_{i+} - \mathbf{r}_{j+}|) + V_e(|\mathbf{r}_{i-} - \mathbf{r}_{j-}|) - V_e(|\mathbf{r}_{i+} - \mathbf{r}_{j-}|) - V_e(|\mathbf{r}_{i-} - \mathbf{r}_{j+}|)] \ , \tag{S4}$$

are the potential energies of interaction between the tip and dipole i and between dipoles i and j respectively, while the positions of the positive and negative charges in the dipoles are given by $\mathbf{r}_{i+}$ and $\mathbf{r}_{i-}$, respectively. The potential energy functions and positions of the atoms are given by

$$V_e(r) = \frac{1}{4\pi\epsilon_0\epsilon r} \ , \tag{S5}$$

$$V_{\mathrm{c}}(r) = V_{\mathrm{c}0} \exp(-r^2/\sigma_0^2) \ , \tag{S6}$$

$$\mathbf{R}_j^{\mathrm{t}} = (X_j, h) \ , \tag{S7}$$

$$X_j = X + b\left(j - \frac{1}{2}(n-1)\right) \ , \tag{S8}$$

$$\mathbf{r}_{i\pm} = \left(ai \pm \frac{1}{2} d \sin\phi_i, \pm\frac{1}{2} d \cos\phi_i\right) \ . \tag{S9}$$

The equations of motion are integrated numerically using a fourth-order Runge-Kutta algorithm.

ADDITIONAL PLOTS AND VIDEO MATERIAL

Here we include some additional plots and video material to further elaborate on the effects shown in Figs. 4 and 5 of the main article.

Figure S1 is for the same system as Fig. 4 of the main article. It shows the lateral force as well as gray scale maps of the kinetic energy for two different field strengths, one close to the transition, where the dipole rotation contributes to the dissipation, and one away from the transition, where it does not. The lateral force shows the typical stick slip behavior with superimposed smaller oscillations. After each slip, energy is transported through the chain and away from the tip by propagating waves. Movies `M1.avi` and `M2.avi` show

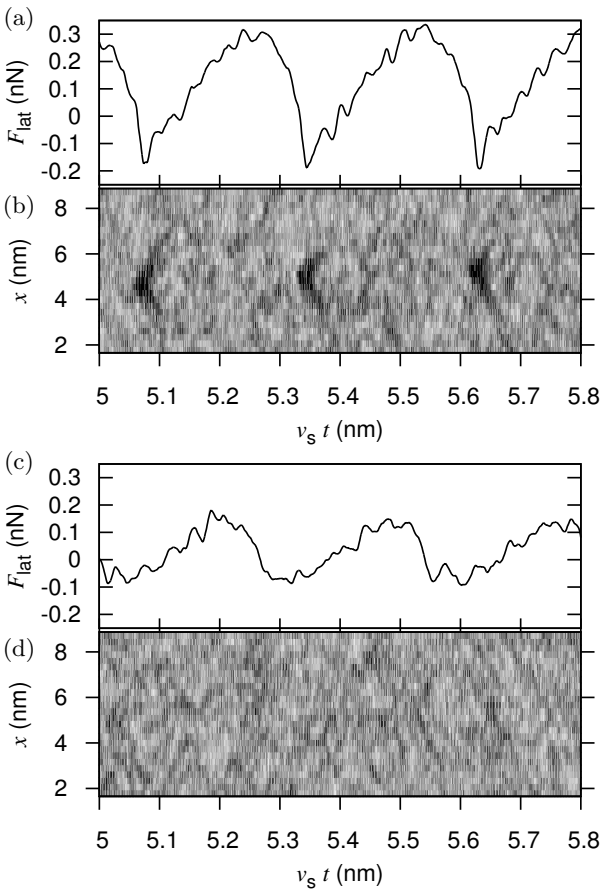

FIG. S1: (a) The lateral force as a function of time for the case of $E_{\mathrm{ext}} = -5$ V/nm (the case of Fig. 4 of the main article). (b) A gray-scale map of the kinetic energy in the dipole rotation as a function of time and position of the dipole for the same simulation as in (a). Dark regions indicate high kinetic energy. During a slip energy is released, and dipole rotation propagate away from the tip, transporting and dissipating energy. (c) The lateral force as a function of time for the case of $E_{\mathrm{ext}} = 0$ V/nm. (d) A gray-scale map of the kinetic energy in the dipole rotation as a function of time and position of the dipole for the same simulation as in (c). In contrast to (b), there are no propagating waves emanating from a slip point in (c). For this field strength, the dipole rotation does not contribute much to the dissipation.

the same simulations, corresponding to Figs. S1(a,b) and (c,d) respectively. The mechanism of dissipation through rapid dipole rotation and rotation wave propagation can be observed in `M1.avi` and Fig. S1b, but not in `M2.avi` and Fig. S1d. The striking propagating rotation waves, which transport energy away from the tip when $E_{\text{ext}} = -5$ V/nm, are missing for other field strengths.