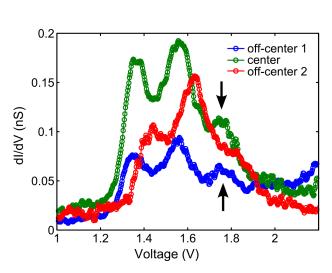
## Switching and charging of a ruthenium dye on Ag(111) – Supplemental material

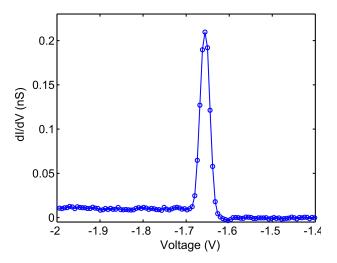
Nadine Hauptmann, $^a$  Christian Hamann, $^a$  Hao Tang, $^b$  and Richard Berndt $^{*a}$ 



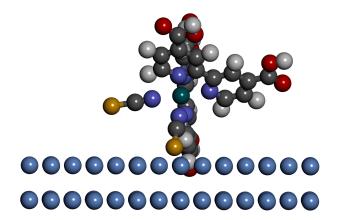
**Fig. S1** Differential conductance dI/dV vs. voltage on an unswitched N3 (Figs. 2(a) and (b)). The data was recorded at the center of the molecules (green) and at two off-center positions (red and blue). A third vibronic peak can be observed (arrow).

## Calculation of $E_0$ and $\alpha$

The energy level  $E_0$  and the fraction  $\alpha$  are calculated from the onsets of P<sup>-</sup> at V<sup>-</sup> and P<sup>+</sup> at V<sup>+</sup> as:  $E_0/e = -V^-\left(\frac{V^+}{V^+-V^-}\right)$  and  $\alpha = \frac{V^-}{V^+-V^-}$ . With the values from Fig. 3(a)  $(V^- = -2.2 \text{ V})$  and  $V^+ = 0.47 \text{ V}$   $E_0 = 0.39 \text{ V}$  and  $\Omega = 0.18$  are obtained.



**Fig. S2** Differential conductance dI/dV vs. voltage of the molecule on which the dI/dV map in Fig. 3(a) was performed. For this molecule we find  $E_0 \sim 240 \,\mathrm{mV}$  from the measured onsets  $V^- = -1.62 \,\mathrm{V}$  and  $V^+ = 0.28 \,\mathrm{V}$ ). The tip-molecule distance is defined by a current of 51 pA and a voltage of  $-2 \,\mathrm{V}$ .



**Fig. S3** Suggested adsorption geometry of N3 at a single step after the switching as viewed from the upper terraces. The step is parallel to the plane of the paper.

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