

Combined Friction Force Microscopy and Quantum Chemical Investigation of the Tribotronic Response at the Propylammonium Nitrate – Graphite Interface

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Supporting Information

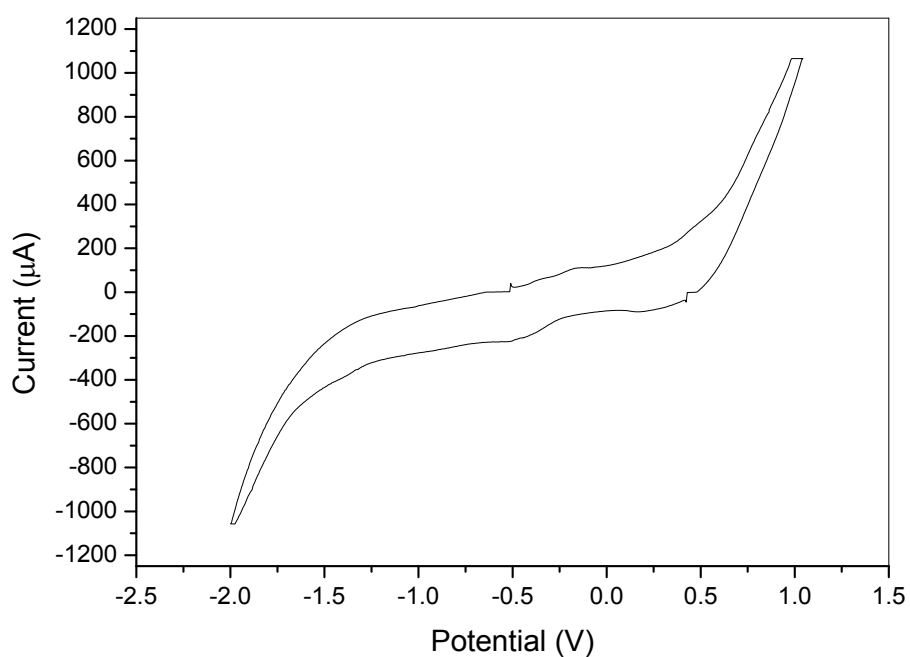


Figure S1. Cyclic voltammogram of PAN at 100 mV.s⁻¹.

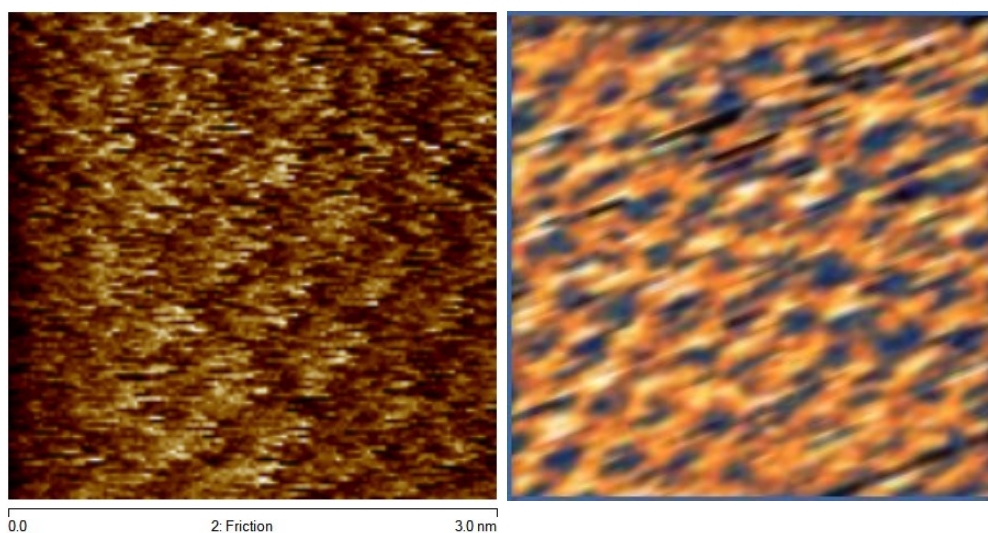


Figure S2. Lateral force image (forward) for the PAN-HOPG interface at 0 V obtained using FFM, and an amplitude modulated AFM image of the same system at the same scale, as described previously.¹ Note that while the features are less clear in the FFM image, the dimensions of the structures, and the rhomboidal symmetry, are consistent.

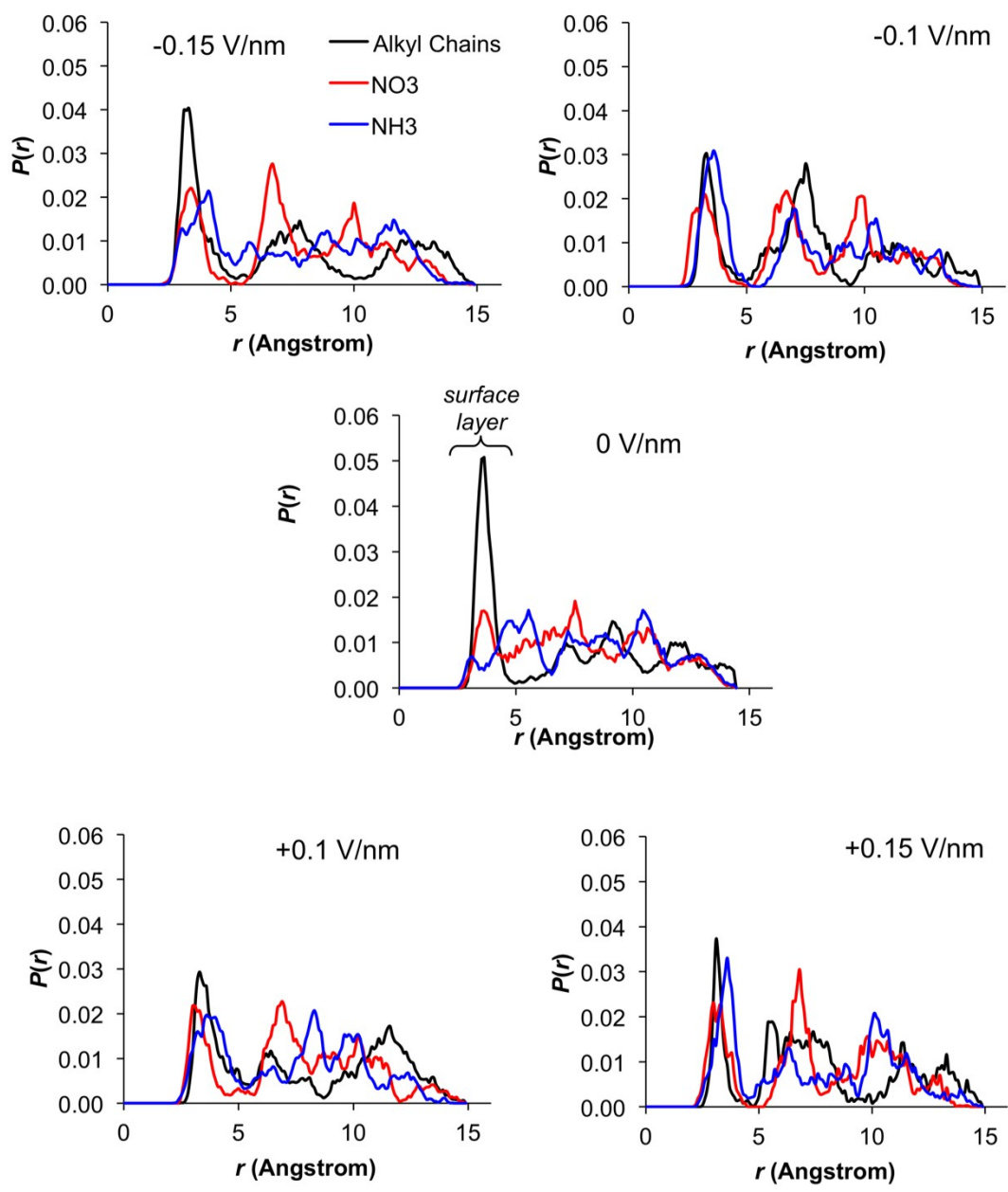


Figure S3. Simulated ion density profiles, normal to the HOPG surface, for the PAN-HOPG interface for applied fields between ± 0.15 V/nm. The surface layer consists of all ions within 5 Å from the HOPG surface. 0 V data is reproduced from reference.¹

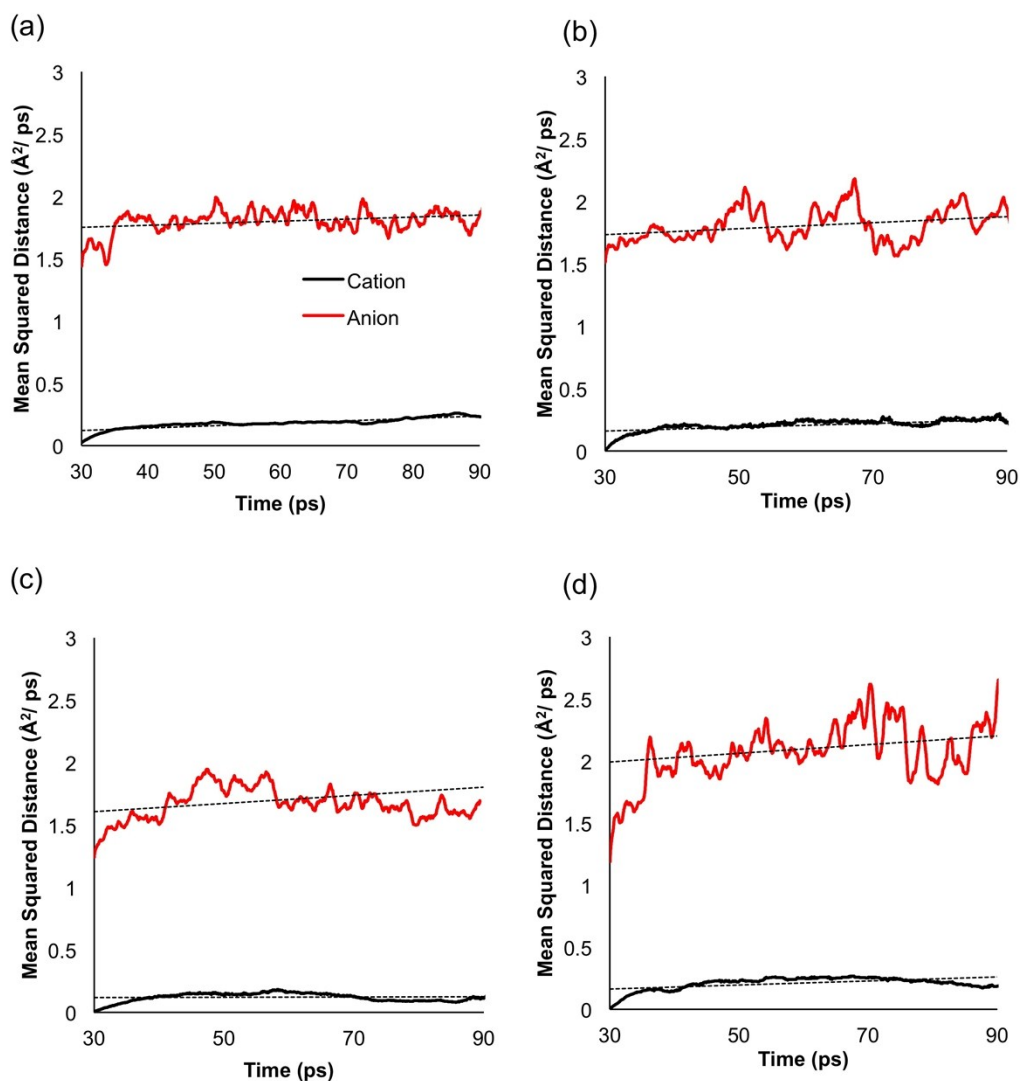


Figure S4. Mean squared displacement of cations and anions in the simulated PAN-HOPG interface at (a) -0.15 V (b) -0.1 V (c) +0.1 V and (d) +0.15 V. Linear regression gives diffusion coefficients ($\times 10^{-1} \text{ m}^2/\text{s}$) of (a) 4.35 ± 0.49 (NO_3^-), 0.93 ± 0.01 (PA^+); (b) 6.70 ± 0.39 (NO_3^-), 1.94 ± 0.03 (PA^+); (c) 15.32 ± 1.43 (NO_3^-), 2.84 ± 0.06 (PA^+); (d) 7.34 ± 1.27 (NO_3^-), 3.19 ± 0.10 (PA^+).

References

1. A. Page, A. Elbourne, M. Addicoat, G. Warr, K. Voitchovsky and R. Atkin, *Nanoscale*, 2014, **6**, 8100-8106.