

Supplementary information for

A Computational Comparison of Ether and Ester Electrolyte Stability on a Ca Metal Anode

Diana Liepinya,^{†,‡} Robert Shepard,[†] and Manuel Smeu^{*,†}

[†]*Department of Physics, Binghamton University, Binghamton, NY*

[‡]*University of Maryland, College Park, MD*

E-mail: msmeu@binghamton.edu

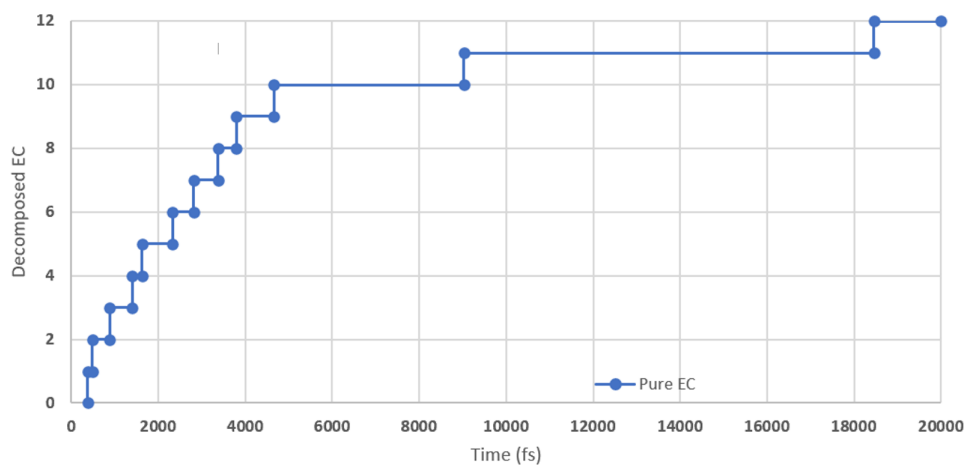


Figure S1: Total number of decomposed EC molecules over simulation run time.

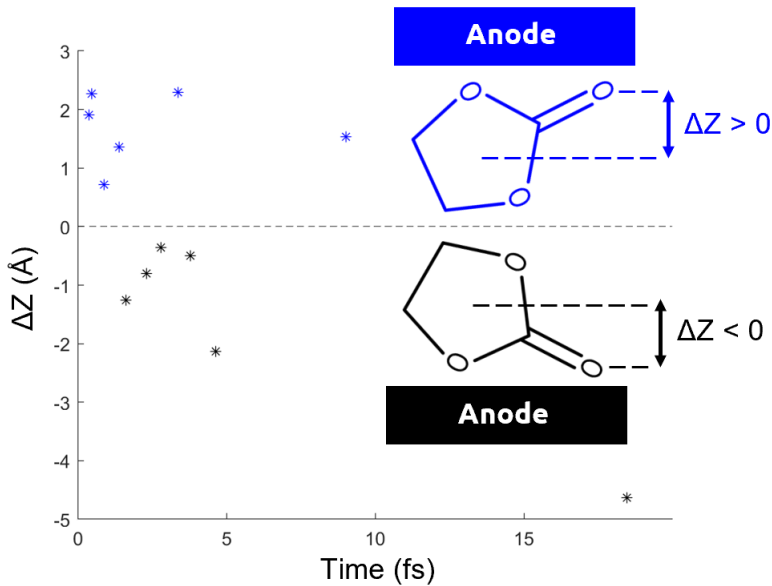


Figure S2: EC orientation at time of decomposition measured as the difference in z position of the carbonyl oxygen and the rest of the molecule. Blue dots are closer to the top surface, while black dots are closer to the bottom surface.

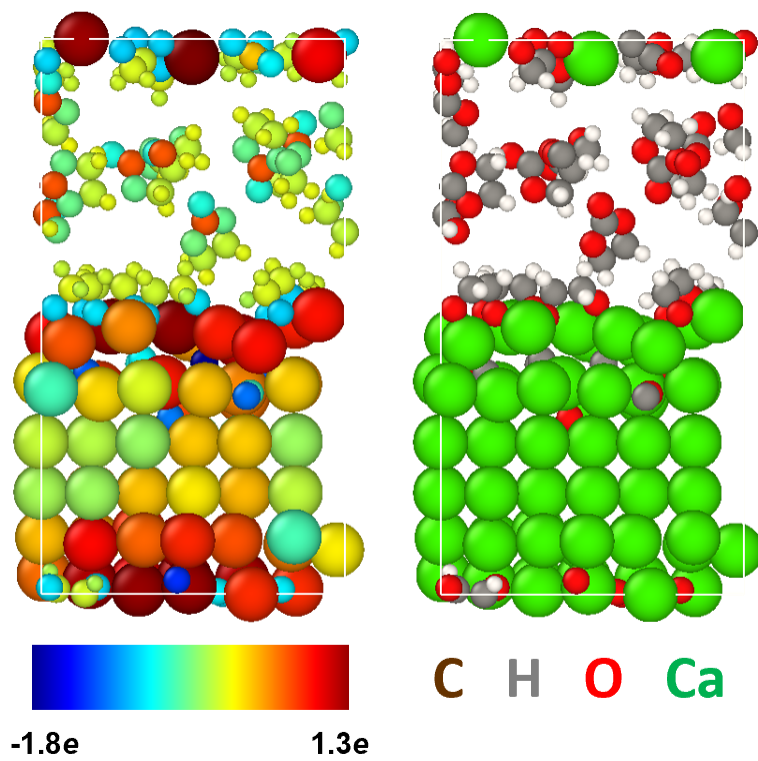


Figure S3: The final step of the pure EC trajectory. The left image is colored according to charge, while the right image provides context for atom type.

