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MD simulations of the effect of grafted charged polymer coatings on electro-osmotic flow OWEN A. HICKEY, JAMES L. HARDEN, University of Ottawa, CHRISTIAN HOLM, University of Stuttgart, GARY W. SLATER, University of Ottawa — Using conventional molecular dynamics simulations with explicit solvent we examine how grafted charged polymer coatings affect the electro-osmotic flow (EOF) in a circular capillary. First and foremost we compare the electro-osmotic properties of the polymer coating to the electrophoretic properties of the polymers which make up the layer. We find that the speed of the bulk electro-osmotic flow is actually slightly higher than the electrophoretic speed of the polymers which make up the coating. We compare this to similar experimental results where the electrophoretic speed was found to be slightly higher than the speed of the EOF generated by the same polymers when used as a coating. We show evidence which suggests that this is due to the incomplete screening of EOF caused by the underlying layers in the polymer coating. We also present other interesting results like the fact that an interface which is electrically neutral can generate a non-zero EOF.

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