Abstract Submitted for the MAR06 Meeting of The American Physical Society

A Molecular Dynamics Study of the Odd-Even Effect in Self-Assembled Monolayers¹ LAWRENCE HERMAN, United States Naval Academy, Midshipman First Class, PAUL MIKULSKI, United States Naval Academy, Physics Department, JUDITH HARRISON, United States Naval Academy, Chemistry Department — Classical Molecular Dynamics has been used to examine the friction in model systems consisting of an amorphous hydrocarbon tip sliding across selfassembled monolayers consisting of well-ordered densely-packed pure linear hydrocarbon chains. An odd monolayer composed of C13 chains is compared against an even monolayer composed of C14 chains at a number of loads. Periodic Boundary Conditions imposed in the horizontal plane are used to model infinite monolayers. The friction of the odd monolayer is seen to be roughly twice as large as that of the even monolayer at all loads. The difference is attributable to the differing orientation of terminal chain groups in odd versus even monolayers. Analysis of net forces exerted by the entire set of tip atoms on individual monolayer atoms lends insight into specific properties associated with the observed frictional difference.

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