Abstract Submitted for the MAR09 Meeting of The American Physical Society

Monolayer solids of short (perfluoro)alkanes on graphite L.W. BRUCH, University of Wisconsin-Madison — Calculations are reported for the relative stability of monolayer solid latices on graphite for  $C_2H_6$ ,  $C_3H_8$ ,  $C_2F_6$ , and  $C_3F_8$ . Triangular, centered rectangular and two-sublattice herringbone lattices are treated. The calculations use all-atom (AA) models and are based on non-bonding interactions formulated for three dimensional dense phases of alkanes and perfluoroalkanes.

L. W. Bruch University of Wisconsin-Madison

Date submitted: 19 Nov 2008

Electronic form version 1.4