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Simulations of the Monolayer Lubricants on Solid Surfaces DOUGLAS IRVING, CLIFFORD PADGETT, SIMON KELLY, DONALD BRENNER, Department of Materials Science and Engineering, North Carolina State University — Lifetimes of moving interfaces in MEMS devices can often be extended by using a thin lubricant coating. These lubricants, however, can have reasonably narrow conditions of temperature and pressure over which they provide effective protection against friction and wear. To gain new insights into the nanoscale properties of monolayer lubricants, we have been carrying out atomic and continuum simulations of several classes of molecular overlayers on metal and semiconductor surfaces under sliding conditions. This talk will focus on recent continuum simulations of benzene on copper and molecular modeling studies of novel bound+mobile lubricant systems (e.g. octadecyltrichlorosilane and tricresylphosphate), where we have characterized heating rates, frictional forces, and the potential for self-healing of these systems over a wide range of temperature and sliding conditions. This work is supported by a MURI grant from the Air Force Office of Scientific Research.

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