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Dynamics of six-member molecular rings adsorbed onto graphite and MgO(100)[1] JOHN Z. LARESE, Oak Ridge National Laboratory and University of Tennessee, PETER YARON, University of Tennessee — Molecular dynamic studies of adsorption of six-member molecular rings (cyclohexane and benzene) onto various substrates (like MgO(100) and graphite) have been undertaken using a commercial modeling package (Materials Studio by Accelyris Software Inc.) that employs central force field potentials. These studies indicate that both systems exhibit rotational translational coupling and strong signs that the translational diffusion is lattice-like on graphite. The cyclohexane rotational motion has a distinct out of plane component coupled to the translational diffusion much like the rolling motion of a wobbly wheel with three hydrogen atoms in "contact" with the substrate plane, while the benzene is more planar. These studies will be compared to results of neutron scattering investigations of the temperature dependance of the dynamics.

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