

**Predicted anomalous behavior of C<sub>60</sub> fullerenes on graphite at low temperature: a new hindered cooperative rotational transition. M.W. Roth<sup>1</sup>, M.K. Balasubramanya<sup>2</sup>, P. Bergmann<sup>1</sup>, M. Karl<sup>1</sup>, M.J. Connolly<sup>1</sup>, and Paul A. Gray<sup>3</sup>, <sup>1</sup>University of Northern Iowa, Department of Physics, Cedar Falls, IA 50614, <sup>2</sup>Department of Physical and Environmental Sciences, Texas A&M University-Corpus Christi, Texas 78412, <sup>3</sup>University of Northern Iowa, Department of Computer Science, Cedar Falls, IA 50614 [rothm@uni.edu](mailto:rothm@uni.edu)**

All – atom molecular dynamics (MD) computer simulations of C<sub>60</sub> fullerene patches adsorbed onto graphite are conducted at various coverages for very low temperatures. There appears to be a hindered tumbling rotational transition through  $T \leq 20$  K seen in the simulations that accompanies dramatic lattice expansion and configurational energy change with temperature in the adlayer. Moreover, the transition is unique in that it appears to be continuous and understandable on the basis of very simple dynamical arguments. The results suggest that such behavior could be present and influential in a wide range of molecules whose dynamical (time averaged) shapes are very close to their static symmetry, in contrast to surface systems with lower symmetry constituents and sharp rotational transitions. The transition is also observed in annealed, percolating adlayers and its dependence on lattice topology is discussed.

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