

Abstract Submitted  
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**The structure of a C<sub>60</sub> monolayer on Ag(111)**<sup>1</sup> RENEE DIEHL, HSIN LI, KELLY HANNA, Penn State University, WOLFGANG MORITZ, University of Munich — The structure of a monolayer of C<sub>60</sub> on Ag(111) was studied using dynamical LEED, the first such study for C<sub>60</sub> molecules. The C<sub>60</sub> monolayer adopts a commensurate hexagonal ( $2\sqrt{3}\times 2\sqrt{3}$ )R30° structure with a nearest-neighbor separation of 10.0 Å. LEED intensities were measured at a sample temperature of 32 K using incident beam energies up to 600 eV. The LEED analysis was performed using conventional methods adapted for large molecular adsorbates, with up to 15 phase shifts to describe the scattering potential. The structure of the monolayer consists of C<sub>60</sub> molecules occupying the top sites with their hexagonal faces down, at a distance of 2.27 Å above the Ag(111) surface. There is an accompanying deformation of the Ag surface that involves the downward displacement of the Ag atoms nearest to the C<sub>60</sub> molecules, consistent with a charge transfer between the surface and the molecule. The C<sub>60</sub> molecules have a significant librational motion about their vertical axes, even at 32 K.

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