Electrostatic Origin of Meandering C60 Chain Formation at ZnPc Interfaces\textsuperscript{1} JANICE REUTT-ROBEY, QIANG LIU, LEVAN TSKIPURI, WEI JIN, JOHN WEEKS, University of Maryland, DANIEL DOUGHERTY, NC State University, STEVE ROBEY, NIST — We present STM investigations of interface-formation and nanophase separation in binary films of zinc phthalocyanine (ZnPc) and C\textsubscript{60} on Ag(111) and Au(111) supports. We report ZnPc:C\textsubscript{60} 1-D and 2-D interfaces with distinctive molecular orientations and unusually low C\textsubscript{60} packing densities. Meandering C\textsubscript{60} chains of single-molecular width arise without registration to the underlying ZnPc template, islanding into a disordered chain phase. These structures are reminiscent of dipole fluids (albeit of single molecular widths!) We present detailed measurements and analysis of C\textsubscript{60} wandering chain formation on ZnPc/Ag (111) and ZnPc/Au (111) substrates. We explore the physical origin of these structures through simulations with a model potential that incorporates short-range C\textsubscript{60} – C\textsubscript{60} attraction and a long-range dipolar repulsion. From simulations of realized structures, we estimate the effective dipole needed for chain formation. DFT calculations on the C60/ZnPc/Ag(111) structure support these conclusions and provide more detailed insight on the electrostatic interactions that drive chain formation.

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