Mechanical Properties of a vdW molecular monolayer at a metal surface: Structural Polymorphism leading to facile compression
DEZHEN SUN, DAEHO KIM, UC Riverside, DUY LE, UC Florida, ØYVIND BORCK, Norwegian University of Science and Technology, KRISTIAN BERLAND, Chalmers University of Technology, KWANGMOO KIM, University of Maryland, WENHAO LU, YEMING ZHU, MIAOMIAO LUO, JON WYRICK, ZHIHAI CHENG, UC Riverside, T.L. EINSTEIN, University of Maryland, TALAT RAHMAN, UC Florida, PER HYLDGAARD, Chalmers University of Technology, LUDWIG BARTELS, UC Riverside — Intermolecular force plays an important role in self-assembly and surface pattern formation. Anthracene and similar unsubstituted arenes attach to a metallic substrate predominantly through van der Waals interaction leading. In this contribution we present images how anthracene on Cu(111) forms a large number of highly ordered patterns that feature a broad array of structural motifs. Density functional theory modeling including vdW interactions allows us to model the energetic of the pattern formation at high fidelity. Moreover, it allows us to deduce the strain energy associated with films of varying coverage. From this work, we obtain the Young’s modulus and Poisson Ratio of a molecular monolayer, which resemble properties conventionally found for porous materials. These patterns are in marked contrast to those found after introduction of functional groups in the molecules, such as carbonyls or thiols.

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