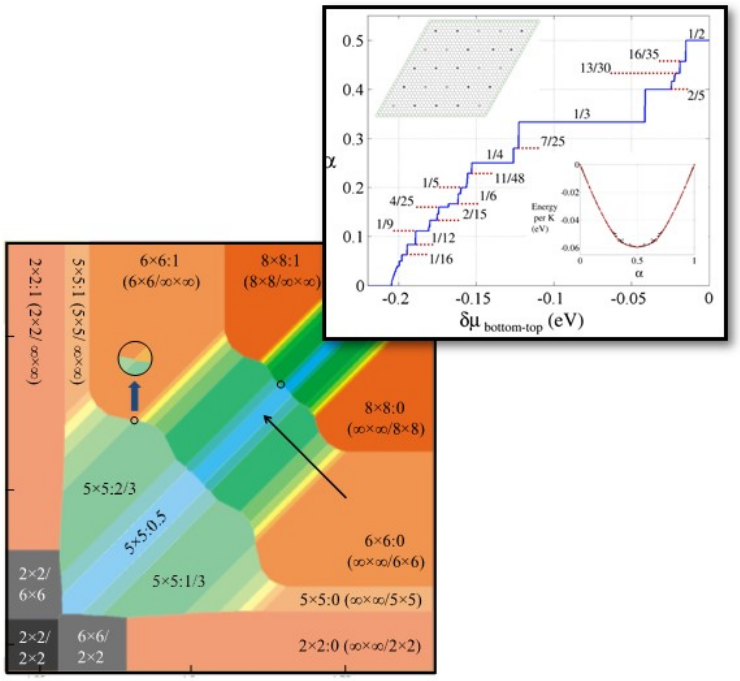
The Pennsylvania State University, N-338 Millennium Science Complex, University Park, PA 16802

MIP: 2D Crystal Consortium DMR-1539916
ARO-MURI W911NF-11-1-0362; DMR-1420620
2018

Dual-sided Adsorption onto 2D

When an atomically thin 2D material is suspended as a membrane so that adsorbed atoms can stick to both sides, these atoms can interact *through* the membrane and thus act as two coupled adsorbate systems, with new properties that are absent in either system alone. Computational modeling in the 2D Crystal Consortium predicts new patterns that emerge, such as an infinite staircase of fractional coverages of opposing sides with simple rational fractions being favored, a so-called "Devil's Staircase." Since adsorbate patterns are possible at different spatial scales, it is possible to obtain parallel staircases with different step heights, and even come arbitrarily close to violating a revered principle of thermodynamics, the Gibbs Phase Rule. These systems provide a new window into the behavior of atoms on surfaces.



DMR DIVISION OF MATERIALS RESEARCH
DIRECTORATE FOR MATHEMATICAL AND PHYSICAL SCIENCES

Tang, Chia, Crespi, Penn State

What Has Been Achieved: A new physical system has been predicted, which couples together two more traditional "surface science" systems by coupling the surfaces on opposite sides of a suspended 2D layer.

Importance of Achievement: This discovery takes the traditional field of surface science – the behavior of atoms on surfaces – and extends it in a new unanticipated direction where two such systems are weakly coupled to each other. This sort of coupling together of previously disparate systems is the domain in which new physics is found.

Unique Features of the MIP That Enabled Project: Access to high-performance computing resources capable of modeling the complex patterns of thousands of adsorbed atoms.

Publication: Y. Tang, C.C. Chia and V. H. Crespi, "Dual-Sided Adsorption: Devil's Staircase of Coverage Fraction ", Phys. Rev. Lett. 120, 056101 (2018).

The 2DCC-MIP is funded by NSF cooperative agreement DMR-1539916.