

# Dynamic Properties and Self-Assembly Mechanisms of Functional Molecules on Insulating Surfaces

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18th International Conference on Non-Contact Atomic Force Microscopy, Cassis, France, **September 7-11<sup>th</sup> 2015**.

Financement : ANR Nanokan  
Audience Internationale  
Conf orale

In this study we used non-contact atomic force microscopy (NC-AFM) and theoretical simulations to study the adsorption, diffusion, film stability, de-wetting, and desorption of functional organic molecules on bulk insulating surfaces at a range of different temperatures. Our results focus on the importance of molecular mobility and flexibility in order to provide insight into the mechanisms that drive self-assembly in these systems.

1,3,5-tri-(4-cyano-4,4 biphenyl)-benzene (TCB) and 1,4-bis(cyanophenyl)-2,5-bis(decyloxy)benzene (CDB) molecules, were synthesized, deposited, and annealed on the KCl(001) substrate at temperatures between 300K to 440K and imaged using NCAFM. DFT calculations were performed to study the adsorption of single molecules and the competing molecule-molecule and molecule-surface interactions for CDB and TCB molecules on KCl(001). These results were used to propose several low energy monolayer structures and parameterize classical force fields for both the TCB and CDB molecules using genetic algorithm methods.<sup>[1]</sup> We then used these force fields in conjunction with molecular dynamics (MD) to study the mobility of individual CDB and TCB molecules at terraces and step edges, the stability of their predicted monolayer configurations, entropic contributions to adsorption energy, and de-wetting.

Combining experimental data and theoretical calculations we demonstrate that the flexibility of the molecule changes its interactions with step edges and the impact this has on the monolayer growth process.

References:

[1] D. Z. Gao, F. Federici Canova, M. B. Watkins, A. L. Shluger, *Journal of Computational Chemistry*, (2015).