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TÉMA

Assembling and Blocking Epitaxial Organic Layers on Si Surfaces

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Because crystalline Si dominates the microelectronics industry, the successful manufacture of hybrid devices, that utilize the optical response or the bio-functional properties of organic materials, faces the imposing challenge of grafting organic functionality onto Si. But Si surfaces are extremely hostile environments for organics and non-covalent synthesis – self-assembling organic layers using surface-confined supramolecular coordination chemistry – is an inappropriate strategy because the strong reaction with the Si surface hinders supramolecular assembly. Consequently, the templating strategies that work well on noble metal surfaces have to be abandoned, and one is forced to develop strategies that employ either Si passivation or direct covalent attachment.

I will demonstrate a strategy, developed using a combination of insight, ab initio calculation and serendipity, for assembling an ordered organic layer on Si(111)-7x7 that uses steric interactions to break the equivalence of the three admissible attachment geometries [1,2]. The methodology is to minimize disorder by sterically hindering nearest neighbor adsorption. Using careful selection of the adsorbate, the surface kinetics can be modified to favor the formation of an ordered molecular array. This approach is illustrated using 1,3,5-trimethyl benzene where three methyl groups provide the steric interaction. To fully understand the ordering processes we used: scanning tunneling microscopy to study site occupancy as a function of coverage, ab initio total energy calculation to study the stability of the binding sites and kinetic Monte Carlo (KMC) modeling to study the ordering kinetics.

I will also demonstrate a methodology for blocking the formation of the organic layers that could, in principle, allow organic layers like mesitylene to be patterned on Si surfaces using a shadow mask or nanostencil [3].

Also, now that we have finally assembled one organic species into an array on Si(111)-7x7, it is natural to ask if these ideas have general utility? Can other organic layers be assembled using this method? I will show some preliminary results from an ab initio, total energy investigation that suggest that we may have identified a second molecular array. However, these results await experimental verification and there are some surprises that reinforce the fact that to graft organics onto Si one must carefully balance several competing interactions.

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References

[1] A. J. Weymouth et al, Phys. Rev. B 84, 165308 (2011).
[2] A. J. Weymouth et al, Chem. Comm. 47, 8031-8033 (2011).
[3] A. J. Weymouth et al, Phys. Rev. B, 85, 155318 (2012).

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