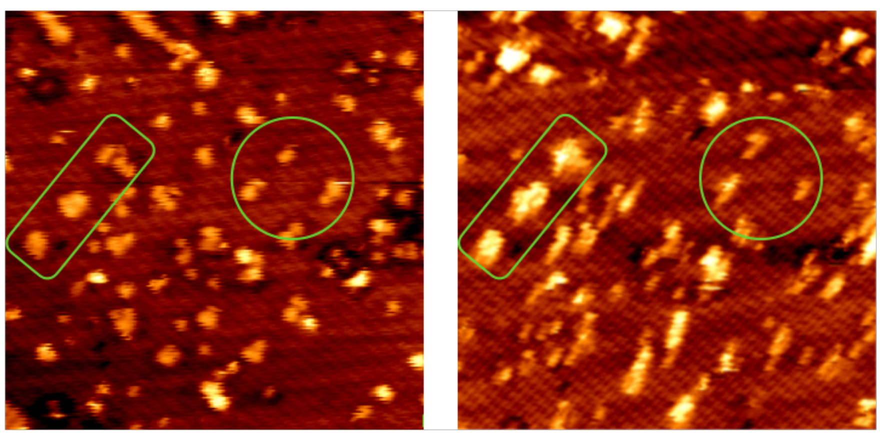
Selective Deposition at the Single-Molecule Limit

J. H. G. Owen* [a], **J. Ballard** [a], **R. Santini** [a], **J. N. Randall** [a] **and J. R. Von Ehr** [a]
[a] *Zyvex Labs LLC, 1301 N. Plano Rd, Richardson, TX 75081, USA*

For applications such as quantum information processing, 2D quantum metamaterials, and single-molecule surface chemistry, the placement and positioning of single molecules is required. This can be achieved using Hydrogen Depassivation Lithography (HDL) to remove H atoms from a Si(001) surface, creating patterns of chemically reactive adsorption sites[1]. For P dopant placement on Si(001), the current process involving a thermal anneal of three adsorbed PH_3 molecules in a 3-dimer pattern results in a P incorporation yield of only 70%, due to an available pathway for PH_3 desorption. One way to avoid this limit is to instead place single PH_3 molecules into 1-dimer patterns, and then remove the H using an STM tip, so as to close the desorption pathway[2]. A similar process is likely to be required for other placed dopants, such as acceptor dopants using B or Al precursors.

We are developing a repeatable process for creating these single-molecule adsorption sites on Si(001):H. For electron donor molecules such as H_2O or PH_3, the required site is a single Si dimer. However, for Trimethyl-Aluminium (TMAl), which is electron accepting, it has been found that adsorption does not occur in 1-dimer patterns, and a larger 2-dimer pattern is required for a single TMAl molecule to adsorb. This may be due to the fact that TMAl adsorbs intact onto the up atom of a buckled dimer, and the required buckling angle (and therefore charge transfer) is not present in a single clean Si dimer surrounded by unbuckled, H-terminated dimers. This talk will discuss the adsorption and incorporation of single molecules of different species to form arrays of dopants of both n and p types.



STM images of 1-2 dimer patterns created on Si(001):H, before (L) and after(R) dosing 20 L TMAl. Adsorption has occurred only on the larger sites, not on the 1-dimer-wide sites.

+ Author for correspondence: * jowen@zyvexlabs.com

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[2] Q. Liu, Y. Lei, X. Shao, F. Ming, H. Xu, K. Wang, and X. Xiao, Nanotechnology, **27**, 135704, (2016).