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Researchers explain how organic molecules bind to semiconductor surfaces

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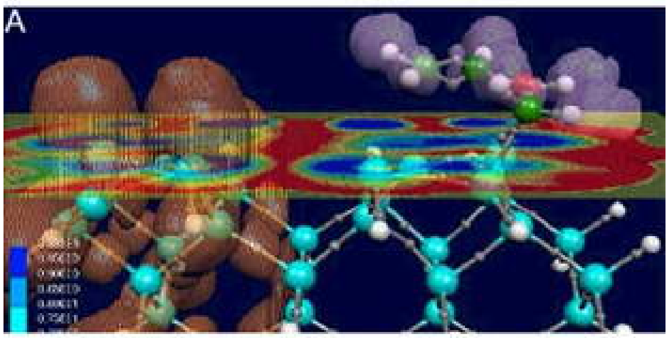

Findings have implications for semiconductor industry

Chemists at New York University have elucidated a mechanism by which organic molecules attach to semiconductor surfaces, a finding that has implications for the semiconductor industry. The industry has sought ways to exploit the attachment process for a variety of purposes. The findings, along with a review of the methodology employed in the study, appear in the latest issue of the Proceedings of the National Academy of Sciences and build on studies published by the same team in the Journal of the American Chemical Society.

Image: Snapshots illustrating the products formed by the addition of an organic molecule (butadiene) to a silicon surface. Green spheres denote *carbon, white spheres denote hydrogen, blue spheres denote silicon, grey spheres and blue surfaces denote centers of high electron density, and red spheres denote local positive charge.*

Mark Tuckerman, an associate professor in NYU's Department of Chemistry and its Courant Institute of Mathematical Sciences, along with graduate student Peter Minary and postdoctoral researcher Radu Iftimie, examined how a butadiene, a particular organic molecule, binds to a particular silicon surface using first-principles computer-based models (Iftimie is now an assistant professor at the University of Montreal, and Minary is a postdoctoral researcher at Stanford University).

The researchers were able to identify four principal products that a butadiene can form when binding to the particular silicon surface they studied. These products had been observed independently in experiments performed elsewhere. More importantly, the researchers were able to rationalize this product distribution with a unified mechanistic picture that addresses a long-standing controversy about the reactions they studied. This mechanism could be used to predict how other organic molecules will attach to the surface and what products might be expected.

The researchers also explored a process of importance in lithography, or surface patterning, wherein they examined how an organic molecule comes off a surface. The process is crucial to the production of computer chips because it requires superimposing surface patterns multiple times with pinpoint accuracy. Specifically, they "reverse engineered" an organic molecule using only their computer model that was found to undergo the reverse reaction--i.e., detachment from the surface--more easily than the original butadiene used in the attachment studies. This finding suggests that the reaction chemistry at the semiconductor surface can be controlled by custom designing or tailoring molecules that exhibit specific desired properties in the reactions they undergo.

Source: New York University