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## Research Highlights

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# Surface chemistry: Hot to trot

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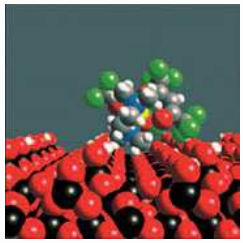
**The motion of a molecule on a hot surface is investigated using molecular dynamics, revealing a regime of fast rolling and vibrational excitation.**

The chemistry that can take place on a solid surface is, in general, dictated by its composition and structure. The effects of harsh conditions such as high temperatures, however, must be considered in processes such as chemical vapour deposition (CVD). Now Gloria Tabacchi of the University of Insubria, Italy, and colleagues from the University of Padua, have used calculations to understand the activation of a CVD precursor molecule on a surface[1]. They simulated the behaviour of an octahedral copper complex on a hydroxylated silica surface at high temperature. The complex bears two pentanedionate ligands and an ethylenediamine ligand and is known to form $Cu_xO$ nanostructures when deposited on a silicon surface.





Using first principles molecular dynamics, Tabacchi and colleagues identified three distinct types of motion. The complex initially undergoes slow back-and-forth diffusion on the surface for a few picoseconds, described by Tabacchi and co-workers as a "bump and rock" motion. This is followed by a regime of very limited movement that lasts for approximately 16 picoseconds during which the complex remains within a very small region on the surface. Subsequently, the behaviour of the complex changes drastically, moving very quickly across the surface in a rolling motion while undergoing large conformational changes.

Tabacchi and co-workers examine how the complex bends and flexes as it passes through these regimes of motion by studying changes in the copper–ligand bond length. They observe that during the fast movement regime the hot surface vibrationally excites the complex producing large bond oscillations and inter-ligand interactions that activate the complex for reaction and increase the chance of reactive collisions.

## Reference

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1. Fois, E., Tabacchi, G., Barreca, D., Gasparotto, A. & Tondello, E. "Hot" surface activation of molecular complexes: insight from modeling studies. *Angew. Chem. Int. Ed.* doi:10.1002/anie.200907312 (2010). | Article

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