Single-molecule study of Heck cross-coupling on surface

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The interaction of organic molecules with metallic structures is particularly important in heterogeneous catalysis where metallic particles or surfaces help to overcome energy barriers of chemical reactions. This concept is specifically important for Heck cross-coupling, which relies on a palladium catalyst to form a carbon-carbon bond between two different reagents [1]. Model heterogeneous catalysis reactions can be investigated by scanning tunneling microscopy (STM) on metal single crystals. The role of active sites could be determined [2, 3], and Heck coupling could be induced thermally [4].
We studied firstly the cross-coupling between vinyl-naphthalene (VN) and different halogenated molecules on a Cu(111) surface by STM at low temperatures (7 K). We analyzed the bond of the de-halogenated molecules to different atomic structures of the copper surface. Then, we investigated the manipulation of a single metal-organic intermediate, and analyzed the products obtained from the thermally induced reaction. In this way we obtained insight into the catalytic activity of the copper surface, and the dependence on the surface morphology.
Subsequently, we deposited palladium nano-islands on a relatively inert Au(111) surface. Thus, the same reaction can be studied on this second substrate, and compared with the performance of the copper substrate. The fundamental understanding obtained with this study might allow a rational design of catalyst materials with controlled stability, activity and selectivity, which operate toward specific cross-coupling.

References

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