Sidharam Pujari

Supervisor(s)	Prof. dr. Cees J. M. van Rijn, Prof. dr. Han Zuilhof
Project	H-terminated Si(111) Modification With trans-enynes: Densely Packed And Highly Stable Monolayers.
Fields of interest	Surface chemistry, High density, Tribology
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Introduction

An enhanced monolayer *quality, faster* monolayer formation and an *increased surface coverage* of the alkenyl monolayers, in combination with the inhibition of oxidation of the silicon substrate due to dense packaging, allows for the implementation of organic monolayers on oxide-free silicon in molecular *electronic and biosensor devices*. Especially in view of the importance of a defect-free monolayer structure and corresponding stability of the monolayer−silicon interface, can this research provide valuable insight.

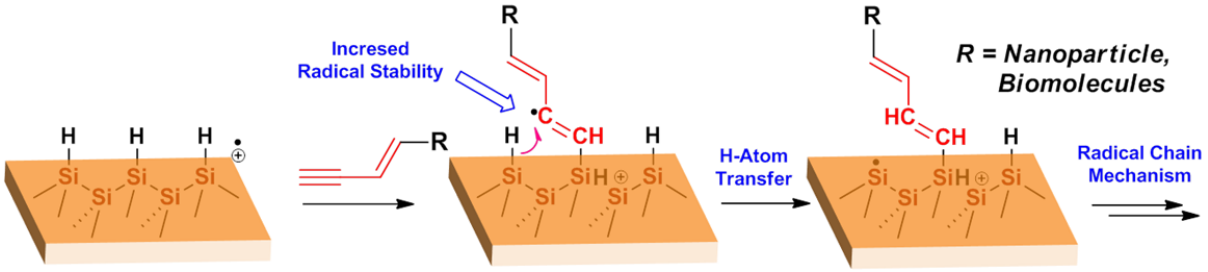

Figure 1: Nucleophilic attack of 3-en-1-ynes to delocalized radical cations at the silicon surface result in the formation of β-carbon radicals. Subsequent transfer of a hydrogen atom from a neighboring Si−H site then results in the formation of a surface-centered radical.

Project description

On H−Si(111), monolayer assembly with 1-ene-ynes yields di-alkenyl monolayers with a Si−C═C-C=C linkage. Five 1-ene-ynes, of length C8, C10, C12, C14 and C16, are going to be synthesized and attached to hydrogen-terminated Si(111) see **figure 1**, to investigate the influence of the chain length on the final monolayer structure. These monolayers are synthesized by a thermal initiation method. The monolayers are going to be characterized with various techniques. The influence of the chain length on the organic monolayers is going to be studied in detail with molecular modeling via PCFF molecular mechanics calculations on periodically repeated slabs of modified Si surfaces. For each monolayer, the packing energies, structural properties, and deformation energies of the Si surfaces for numerous substitution percentages and substitution patterns will be determined.

References

1. Bart Rijksen, Sidharam P. Pujari, Luc Scheres, Cees J. M. van Rijn, J. E. Baio, Tobias Weidner, and Han Zuilhof *Langmuir* **2012** *28* (16), 6577-6588

2. Yan Li, Steven Calder, Omer Yaffe, David Cahen, Hossam Haick, Leeor Kronik, and Han Zuilhof *Langmuir* **2012**, 28 (26), 9920–9929 (Cover image)