

A study of Stereochemical Recognition of Chiral Molecules Investigated by STM-Based Techniques

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The combination of a scanning probe microscope with a photon detector and a Raman spectrometer, referred to as a tunneling-electron-induced light emission (STM-LE) and a tip-enhanced Raman scattering spectroscopy (STM-TERS), is quite attractive and useful to explore the optical properties and chemical analysis of nanomaterials beyond the optical diffraction limit.

In this study, we performed the STM observation to elucidate structural configuration of chiral molecules adsorbed on the metal substrates accompanied with their optical and vibrational properties using our laboratory-built STM-LE and STM-TERS systems¹⁻⁴. As for the chiral molecules, we used racemic-mixture and enantiopure molecules of the chiral PTCDI (*N,N'*-Di-*n*-octyl-3,4,9,10-perylenetetracarboxylic Diimide) and thiaheterohelicene and their derivatives. We clearly observed the high resolution STM images for the chiral molecular assemblies, leading to the important perspective of stereochemical chiral recognition based on the formation of ordered molecular structures combined with their optical and vibrational characterizations. Theoretical calculation based on a density functional theory and a molecular dynamics simulation successfully identified the formation mechanism of the molecular self-assemblies in the chiral recognition schemes.⁵ Moreover, we attempted to investigate the optical dissymmetry of chiral PTCDI molecules using STM-LE measurement, and that of helicene derivatives using the STM-TERS measurements for evaluating the optical activity and identifying the enantiomers of the chiral molecules at a molecular scale.

References

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Supplementary information

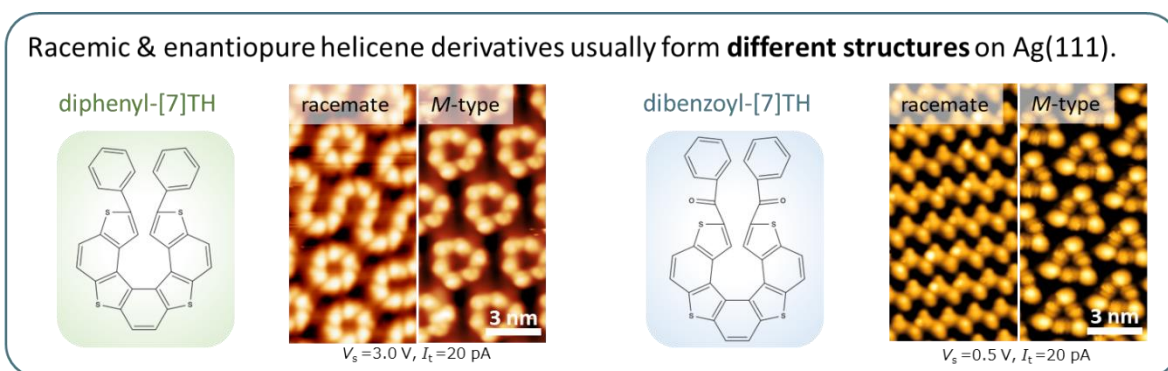


Figure 1. The schematic models of two helicene derivatives (diphenyl-[7]TH and dibenzoyl-[7]TH) and their corresponding STM images. All of the molecules are deposited on Ag(111) surfaces in UHV and STM measurements were performed at 80 K using Ag tips. In the images each protrusion is corresponding to one molecule. Both helicene derivatives show the different type of self-assemblies between racemic mixture and enantiopure (M-type) molecules.