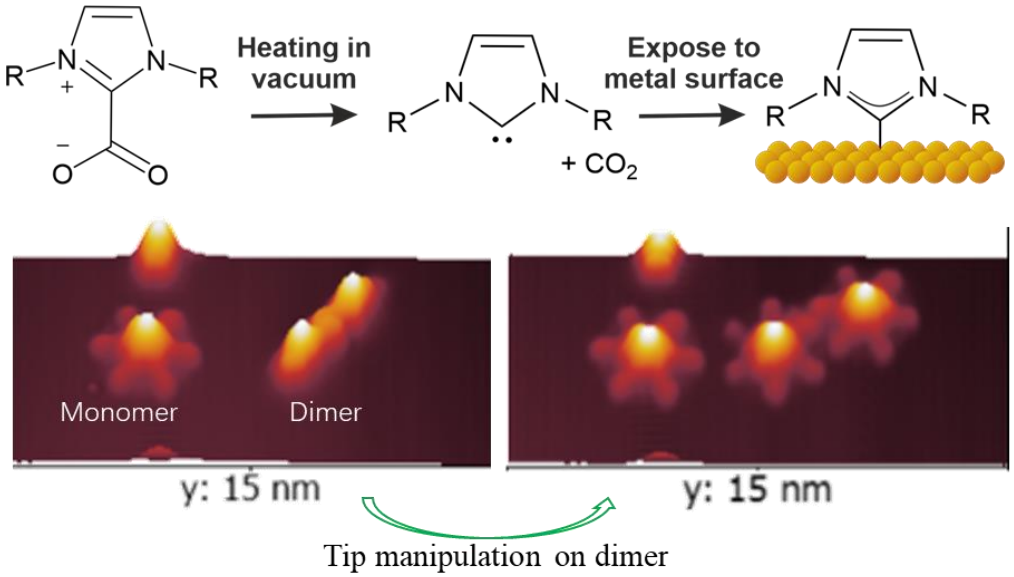
On Surface Behaviors of N-heterocyclic Carbene

As a novel surface modifier, N-Heterocyclic carbene (NHC) can effectively functionalize the physical and chemical properties of the material surface. The development of new methods for controllable self-assembly to achieve precise control of the charge transfer at molecular structures and surface interfaces is a core technical point in the fields of photodetectors, energy and catalysis. Here we report the on-surface behaviors of both monomeric NHCs[1-2] and its polymers[3] on metal surfaces. NHCs have been rationally designed, synthesized and deposited on metal surfaces under UHV conditions. we have realized the controllable regulation of the self-assembly of the electron-rich cyCAAC[2], for the first time, by ultra-high vacuum and low-temperature scanning tunneling microscope (LT-STM), X-ray photoelectron spectroscopy and density functional theory (DFT). The controllable self-assembly has been achieved via tuning the functional groups in NHC. Through the accurate analysis of the stereoisomerism, the surface adsorption and diffusion kinetic model, the high-precision characterization of the surface microstructure of the NHC with ballbot configuration has been achieved. Furthermore, via the delicate balance between mobility and polymerization rate, we successfully synthesize the ballbot-type NHC polymers[3]. These NHCs monomers and their derivatives provide new opportunities in the fields of nanoelectronics, surface functionalization, and catalysis.



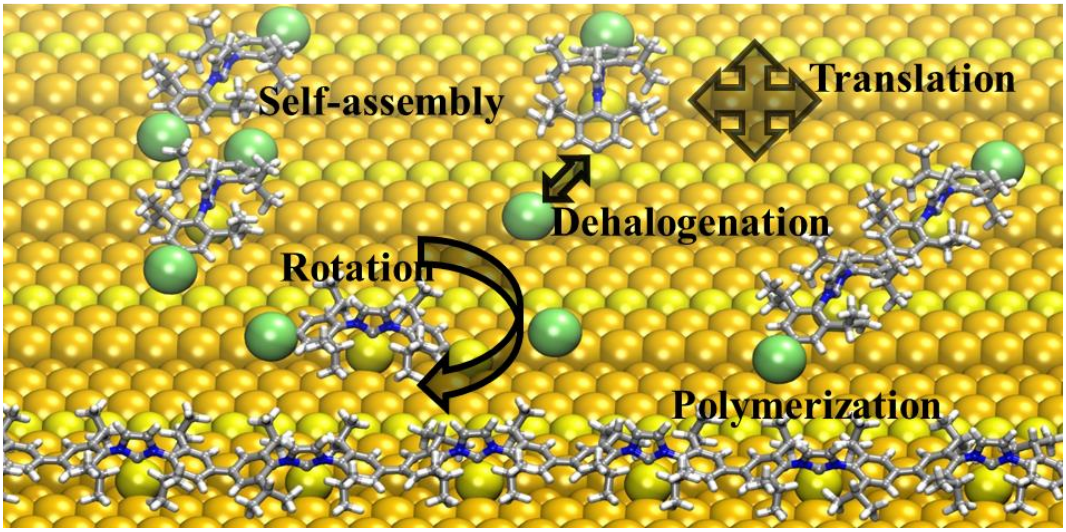


Figure caption: Chemical structures[4], deposition methods and surface manipulations of N-heterocyclic Carbene

References

[1] Jindong Ren+, Matthias Freitag+, Christian Schwermann+, et al. *Nano Lett.* **2020, 20:** 5922-5928

[2] Jindong Ren+, Matthias Freitag+, Yuxiang Gao+ et al. *Angew. Chem. Int. Ed.* **2022, 61:** e202115104

[3] Jindong Ren, Maximilian Koy, Helena Osthues, Bertram Schulze Lammers, Christian Gutheil, Marvin Nyenhuis, Qi Zheng, Yao Xiao, Li Huang, Arne Nalop, Qing Dai, Hong-Jun

Gao*, Harry Mönig*, Nikos L. Doltsinis*, Harald Fuchs*, Frank Glorius*. On-surface synthesis of ballbot-type N-heterocyclic carbene polymers. Nature Chemistry.**2023,** In press.

[4] Gaoqiang Wang. et al. Ballbot-type motion of N-heterocyclic carbenes on gold surfaces. Nature Chemistry 9, 152-156 (2017).