

Observation of proton tunneling in hydrogen-bonded organic 1D molecular chains on Au(111)

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One-dimensional structures offer a rich ecosystem for realizing quantum states with potential application for advanced information technologies. Surface confined molecular self-assembly is one avenue for creating 1D systems, where the extant structure is controlled by the precursor shape, and functional group interlinking chemistry.

Here we study self-assembled 1D chains of zwitterionic molecule 2,5-diamino-1,4-benzoquinonediimines (DABQDI) [1] on Au(111) in ultrahigh vacuum at 5K using combined scanning tunneling and non-contact atomic force microscopies (STM/ nc-AFM) supported by theoretical analysis. Sub-molecular resolution achieved with a CO-functionalized tip hints structural information, specifically regarding the hydrogen bonds linking the precursor units.

To study how this proton tunneling we are using QM/MM techniques [2] to calculate the free energy barrier of the proton transfer at different temperatures. This free energy profile reveals a decreasing barrier with lower temperatures due to the reductions of the vertical movement of the atoms. We also study with Path Integral Molecular Dynamics [3] the proton transfer revealing a deep tunneling regime and a cooperative effect in the proton transfer.

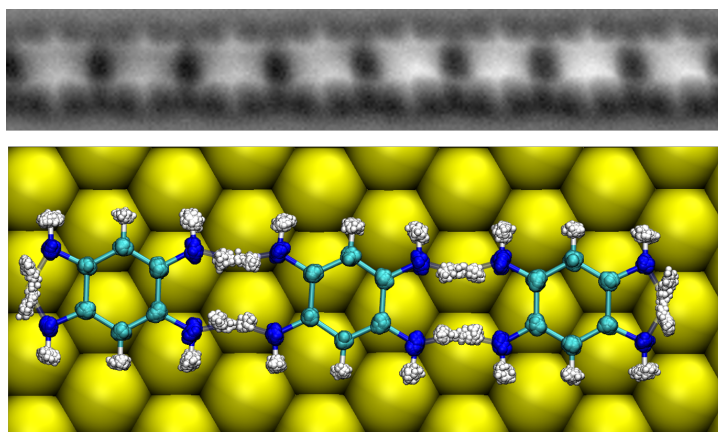


Figure: experimental images of the hydrogen bond chain and the transition state of the proton transfer with PIMD.

References

1. S. Pascal, O. Siri, Coordination Chemistry Reviews, Volume 350, 178-195, (2017)
2. J. I. Mendieta-Moreno et al, J. Chem. Theory Comput. 10, 2185–2193, (2014)
3. Kapil et al., Comp. Phys. Comm. 236, 214–223 (2018)