Quinone-based 1D molecular chains on surfaces: magnetism and nuclear quantum effects

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Low dimensional materials offer very interesting material and physical properties due to reduced dimensionality. At present, 2D materials are the focus of attention. However, 1D systems often show far more exotic behavior due to reduced dimensionality enhancing substantially quasiparticle interactions. However, synthesis of purely 1D molecular systems still remains elusive. In this talk, we will explore on-surface chemistry using 2,5-diamino-1,4-benzoquinonediimines (2HQDI) precursor [1], which offers interesting playground for growing molecular chains of distinct chemical character.

In first part of the talk, we will present formation of hydrogen-bonded 2HQDI molecular chains on Au(111) surface. We will discuss a significant influence of nuclear quantum effects on structural, mechanical and electronic properties of these 2HQDI molecular chains. Namely, we demonstrate that the presence of concerted proton motion not only enhances significantly the cohesive energy of intermolecular hydrogen bonds but it also causes emergence of new electronic states located at the edges [2].

In the second part, we introduce on-surface synthesis of 1D coordination π-d conjugated polymers, achieved by co-deposition of 2HQDI molecular precursor and various transition metals (Fe, Co, Ni, Cr, Cu) atoms on metal surfaces under UHV conditions [3]. This route results in formation of flexible coordination polymers with length up to hundreds of nanometers. We characterize physical and chemical properties by means of low temperature UHV scanning probe microscopy supported by theoretical simulations. We will discuss distinct coordination of transition metal and corresponding atomic, electronic and magnetic structure [4]
Finally, we will demonstrate fully reversible multiconfigurational light-driven spin crossover switches in a single π-d organometallic Co-QDI chain suspended between two electrodes. The external light enables us to realize reversible spin cross over between low and high-spin states of individual cobalt centers within the chain.

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[2] A. Cahlik et al ACS Nano 15, 10357 (2021).
[3] V.M. Santhini et al, Angew. Chem. Int. Ed. 60, 439 (2021).
[4] Ch. Wackerlin et al, ACS Nano (2022) DOI: 10.1021/acsnano.2c05609