Quantum simulator to emulate lower dimensional molecular structure

E. Sierda[1], X. Huang[1], D. Badrtdinov[1], B. Kiraly[1,2], E. Knol[1], G. Groenenbaum[1], M.I. Katsnelson[1], M. Rösner[1], D. Wegner[1] and A.A. Khajetoorians[1]

[1] *Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands*
[2] *School of Physics and Astronomy, University of Nottingham, Nottingham, United Kingdom*

e.sierda@science.ru.nl

Designing materials with tailored physical and chemical properties requires a quantitative understanding of interacting quantum systems. In order to provide predictability, a promising route is to create bottom-up platforms, where the electronic properties of individual and interacting atoms can be emulated in a tuneable manner. Here, we present a solid state quantum simulator based solely on patterned Cs atoms on the surface of semiconducting InSb(110), a system characterized by a dilute two-dimensional electron gas decoupled from the substrate's bulk bands. We use this platform to create electron traps that emulate artificial atoms by precisely positioning Cs atoms using atom manipulation in scanning tunneling microscopy (STM). Localized states of such artificial atom are expected based on ab initio calculations and confirmed by probing with scanning tunnelling spectroscopy (STS). These artificial atoms serve as building blocks to realize artificial molecular structures with different orbital symmetries which are probed by spatially dependent tunneling conductance maps. We find bonding and anti-bonding states for coupled dimers of artificial atoms and orbitals of higher symmetries (π orbitals) for a linear assembly of a few artificial atoms. Based on these artificial orbitals and various atomic patterns, we emulate the structure and orbital landscape of well-known planar organic molecules, including antiaromatic molecules. Presented results validate this new quantum simulator platform and prove its high tunability. [1]

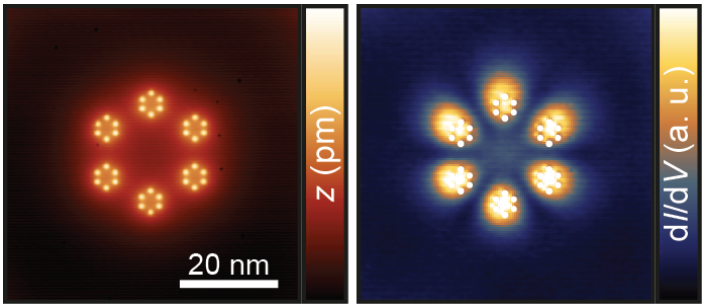

Fig. 1. STM image of artificial atoms in hexagonal arrangement resembling benzene structure and spatial distribution of one of its orbitals probed in the experiment.

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