Original experimental data and code for the Paper "Quantum spins and hybridization in artificially-constructed chains of magnetic adatoms on a superconductor“

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This directory contains the experimental data and the code used in the paper "Quantum spins and hybridization in artificially-constructed chains of magnetic adatoms on a superconductor“. This is a short guide how to handle the files in this directory.

The data files (.sxm and .dat) can be opened and browsed with SpectraFox [**?**]. The .sxm-files can further be opened with WSxM [**?**]. Both programs are free open-source software solutions for managing, processing, and evaluating scientific scanning probe microscopy (SPM) data files. SpectraFox can be downloaded at https://www.spectrafox.com/. WSxM can be downloaded at http://wsxm.eu/.

Data of Figure 1

```
Raw data files:
(a)
\Figure1\image_097.sxm
(b)
\Figure1\image_567.sxm
\Figure1\image_583.sxm
(c)
Topographies are the same data as in Figure 3 a-c (smaller scale).
(d)
\Figure1\image_646.sxm

All topographies have been plane corrected and smoothed in WSxM.
```

Data of Figure 2

```
Raw data files:
(a)
Figure2\cloud_No02_001.dat
Figure2\cloud_No02_002.dat
(b)
Figure2\image_025.sxm
Figure2\line_No02_001-045.dat
(c)
Figure2\cloud_No02H_001.dat
Figure2\cloud_No02H_002.dat
Figure2\cloud_No02H_003.dat
(d)
Figure2\image_031.sxm
Figure2\line_No02A_001-052.dat
(e)
Figure2\cloud_No02L_001.dat
Figure2\cloud_No02L_002.dat
Figure2\cloud_No02L_003.dat
Figure2\cloud_No02L_004.dat
(f)
Figure2\image_006.sxm
Figure2\line_No02B_001-061.dat
(g,h)
Close-ups from (f).

All topographies have been plane corrected and smoothed in WSxM.

All dI/dV spectra were offset corrected with respect to the
corresponding substrate spectrum and then normalized to [4.5mV,5.0mV].
```

Data of Figure 3

```
Raw data files:
(a)
Figure3\image_025.sxm
Figure3\dIdV_No02_001.sxm
(b)
Figure3\image_031.sxm
Figure3\dIdV_No02_002.sxm
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(c)
Figure3\image_045.sxm
Figure3\dIdV_No02_003.sxm
(d)
Different zooms from (a,b).

All topographies have been plane corrected and smoothed in WSxM.

dI/dV-maps are calibrated to conductance units (nS) using a reference spectrum recorded with same lock-in parameters.

(e)
The positions of the resonances were obtained from deconvolved spectra as described in the Supplementary Information.

Data of Figure 4

Raw data files:

(a)
Figure4\image_058.sxm
Figure4\line_No02C_001-072.dat
(b)
Figure4\image_068.sxm
Figure4\line_No02D_001-082.dat
(c)
Figure4\image_077.sxm
Figure4\line_No02E_001-091.dat
(d)
Figure4\image_238.sxm
Figure4\grid_No02D_081-160.dat
(e)
Figure4\image_035.sxm
Figure\grid_No02E_091-180.dat
(f)
Figure4\image_039.sxm
Figure4\grid_No2F_101-200.dat
(g)
Figure4\image_276.sxm
Figure4\grid_No2G_111-220.dat
(h)
Figure4\image_303.sxm
Figure4\grid_No02H_121-240.dat

All topographies have been plane corrected and smoothed in WSxM.

All dI/dV spectra were offset corrected with respect to the corresponding substrate spectrum and normalized.

Data of Figure 5

Raw data files:

(a)
Figure5\line_No02N_001-280.dat
dI/dV spectra were offset corrected and then normalized.

(b)
Figure5\image_470.sxm
The topography has been plane corrected and smoothed in WSxM.

(c)
FFT filtering processing (performed in WsXM):
1) redimension Topography to 512x512 pixels
2) recalibrate z to have positive z-values only
3) filtered with ellipse window

Data of Figure 6

Raw data files:

(a)
Figure6\image_662.sxm
The topography has been plane corrected and smoothed in WSxM.

(b)
FFT filtering processing (performed in WsXM):
1) redimension Topography to 256x1536 pixels
2) recalibrate z to have positive z-values only
3) filtered with ellipse window

(c)
Figure6\line_No02O_001-531.dat
dI/dV spectra were offset corrected and then normalized.

SUPPLEMENTARY INFORMATION

Code for Figure S1 and S2

Files:
FigureS1_S2\code_for_fig_s1_s2
Mathematica notebooks used to generate the data for Figs. S1 and S2. We used Mathematica version 11.2.

FigureS1_S2\code_for_fig_s1_s2\low_energy_exact_diagonalization_spin_half.m
contains functions for constructing the sparse low energy hamiltonian, diagonalizing it, and for calculating the spectral function

FigureS1_S2\code_for_fig_s1_s2generate_data_for_fig_s1_and_s2.nb
imports the above functions and calculates data for the plots

FigureS1_S2\code_for_fig_s1_s2\make_fig_s1_and_s2.nb
makes the plots

Data of Figure S3

Raw data files:

(a)
FigureS3\image_191.sxm
The topography has been plane corrected and smoothed in WSxM.

(b,c)
Close-ups from (a).

Data of Figure S4

Raw data path:

(a)
FigureS4\image111.sxm
Topography of atom at 1.1K.
The topography has been plane corrected and smoothed in WSxM.

(b)
FigureS4\cloud#07_8K_kondo_001-005.dat
FigureS4\substrat_8K_kondo_001,002.dat

The dI/dV spectrum has been (after appropriate offset correction) averaged between the five spectra stated above.

Due to thermal drift when heating up the system from 1.1K to 8K the
coordinates of the topography in (a) and the spectrum in (b) do not coincide.
It was assured that (b) contains the dI/dV spectrum of the atom shown in (a)
by tracing the atom during the warm-up process.

Data of Figure S5

Data files:
(a)
Deconvolved spectra of Fig. 2a,c,e:
FigureS5\cloud_No02_001.txt
FigureS5\cloud_No02_002.txt

FigureS5\cloud_No02H_001.txt
FigureS5\cloud_No02H_002.txt
FigureS5\cloud_No02H_003.txt

FigureS5\cloud_No02L_001.txt
FigureS5\cloud_No02L_002.txt
FigureS5\cloud_No02L_003.txt
FigureS5\cloud_No02L_004.txt

(b)
Data reproduced from Figure 2f.

(c)
FigureS5\line_No02B_050.txt

The .txt-files for Figure S5a contain all original data columns and the following additional columns: ”Smoothed data“ and ”sampleDoS“. The latter being the deconvolved dI/dV spectrum.

The .txt-file for Figure S5c contains all original data columns plus the following colums:

- "symmetrized_data": symmetrized sample DoS (w.r.t. zero energy)
- "Fit": total fit (sum of six Gaussian curves, i.e. 3 for the α- and 3 for the β-states)
- the six individual Gaussian curves of the 3 α- and 3 β-states which are labeled "A1", "A2", "A3", "B1", "B2" and "B3"

Data of Figure S6

```
Raw data files:

(a)
FigureS6\image_500.sxm

(b)
FigureS6\image_505.sxm

(c)
FigureS6\image_500.sxm
FigureS6\cloud_No02+A_001-062.dat

(d)
FigureS6\image_505.sxm
FigureS6\cloud_No02+B_001-064.dat

All topographies have been plane corrected and smoothed in WSxM.
dI/dV spectra were offset corrected and then normalized.
```

Data of Figure S7

```
This figure presents additional dI/dV channels contained in the same raw data files as in Figure 3.

Raw data files:
(a)
Figure3\image_025.sxm
Figure3\dIdV_No02_001.sxm
(b,d)
Figure3\image_031.sxm
Figure3\dIdV_No02_002.sxm
(c,e)
Figure3\image_045.sxm
Figure3\dIdV_No02_003.sxm

All topographies have been plane corrected and smoothed in WSxM.

dI/dV-maps are calibrated to real units.
```

Data of Figure S8

```
Raw data files:

(a)
FigureS8\image_058.sxm
FigureS8\dIdV_No02_004.sxm

(b)
FigureS8\image_068.sxm
FigureS8\dIdV_No02_005.sxm

(c)
FigureS8\image_078.sxm
FigureS8\dIdV_No02_006.sxm

(d)
FigureS8\image_238.sxm
FigureS8\dIdV_No02_007.sxm

All topographies have been plane corrected and smoothed in WSxM.

dI/dV-maps are calibrated to real units.
```

Data of Figure S9

```
Raw data files:
(a)
FigureS9\image_276.sxm
FigureS9\dIdV_No02_008.sxm

(b)
FigureS9\image_303.sxm
FigureS9\dIdV_No02_009.sxm
```

```
All topographies have been plane corrected and smoothed in WSxM.

dI/dV-maps are calibrated to real units.
```

Data of Figure S10 and S11

```
Raw data files:

FigureS10_S11\image_472.sxm
FigureS10_S11\dIdV_No02_011.sxm

The topography has been plane corrected and smoothed in WSxM.

dI/dV-maps are calibrated to real units.
```

Data of Figure S12

```
Raw data files:

FigureS12\image_643.sxm
FigureS12\dIdV_No02_015.sxm

The topography has been plane corrected and smoothed in WSxM.

dI/dV-maps are calibrated to real units.
```

Data of Figure S13

```
Raw data files:

FigureS13\dIdV_No02_017.sxm (topography)
FigureS13\dIdV_No02_016.sxm (dI/dV map)

The topography has been plane corrected and smoothed in WSxM.

dI/dV-maps are calibrated to real units.
```

[] M. Ruby, SoftwareX **5**, 31 (2016).

[] I. Horcas, R. Fernández, J. Gomez-Rodriguez, J. Colchero, J. Gómez-Herrero, and A. Baro, Rev. Sci. Instrum. **78**, 013705 (2007).