Original data files and documentation of data analysis for:
Diode effect in Josephson junctions with a single magnetic atom

Eight folders are uploaded to Refubium.

The raw data files are contained in five separate folders: **RawData-Main**, **RawData-Sup-Jos_CrAll**, **RawData-Sup-Jos_MnAll**, **RawData-Sup-Jos_PbAll**, and **RawData-Topo_dIdV**. The data included in the main text of the manuscript is found in **RawData-Main** while the extended data files are located in the folders starting with **RawData-Sup-**.

In the **Analysis** folder the Python code that was used to analyze the Raw data is located. The exact procedure is explained below.

In the folder **Results** the intermediate results of the python code are saved so that they can be further analyzed as described below.

The **TheoSim** folder holds the code for simulating the IVs curves used in the manuscript. More Details are found below.

For the smooth operation of the code, it is advisable to save the **Analysis** and **Results** folder in a folder called **DataAnalysis**. In **DataAnalysis** also create a subfolder called **RawData**. To this folder **RawData-Main** should be extracted. Rename this folder to **Main**. In **DataAnalysis/RawData** create a folder called **Sup**. All folders on Refubium starting with **RawData-Sup-** should be extracted here. Also rename these folders according to their names to **Jos_CrAll**, **Jos_MnAll**, **Jos_PbAll**, and **Topo_dIdV**. This is necessary because the Python codes need to access the data from the **RawData** and **Results** folder. If the directories are chosen differently, all directory paths need to be adjusted in the Python codes to point at the right location of the data to be analyzed as indicated in the documentation.

In the following text the assignment of the data to the different figures and python codes is documented according to the following directory-trees as indicated above:

DataAnalysis/RawData/Main → contains files and folders from **RawData-Main.zip**

DataAnalysis/RawData/Sup → contains files from all folders starting with **RawData-Sup-[…].zip**

DataAnalysis/Analysis → contains files and folders from **Analysis.zip**

DataAnalysis/Results → contains files and folders from **Results.zip**

General information for analysis of the Josephson data:

The Josephson junction data is analyzed in two steps. First, the switching I_{sw} and retrapping currents I_{re} and the phase diffusion conductance G_{PD} are extracted from the IV data. The results are further analyzed and displayed in the manuscript in a second step. As the Python code needs to access the data for example in the **RawData** folder and needs to save it in another location it is advisable to save all provided folders in the same folder called **DataAnalysis**.

Step 1:
Analysis\ExtractSwitchRetrap\JosephsonSwitchRetrap.py

A self-written python code is used to extract I_{sw}, I_{re} and G_{PD} (the slope in the trapped state) from the measured data for statistical analysis. The code saves intermediate steps of the data processing protocols. In principle, the code can also be used to correct for bias offset and piezo creep, though the piezo creep correction was not used in this manuscript. In the end I_{sw}, I_{re}, G_{PD} and the time of the

measurement is saved in .txt files separated for forward and backward sweep for each individual measurement run (here between 500 and 2000 sweeps). In a second .txt file the averaged data as a summary of each run is collected to easily compare different measurement runs. Details for using the code are given below and can be found in the comments directly in the code. Note that while JosephsonSwitchRetrap.py is the executable file for this code all parameters are set in **CONSTANTS.py**.

Step 2:

From the results of **Step 1** secondary Python programs are used to analyze the data further and plot it in the way presented in the manuscript. These programs will use the output generated by the first Python code. Details for using the code are given below and can be found in the comments directly in the code.

These are the executables for the different plots. Note that directories might need changing when executing the code.

The following codes were used to create figures from the results of **JosephsonSwitchRetrap.py**:

*Analysis**Plotting*\...

Main text:

Figure 1 b)-d):	*VI**VI-curves*
Figure 2:	*IswIreGPD**IswIre_Gpd.py*

Extended Data:

Extended Data Figures 1-4:	*Histo**Histo_plot.py*
Extended Data Figures 5 & 6:	*IswIreGPD**IswIre_Gpd.py*

General information for all other analysis:

dIdVs and IVs in the voltage bias regime are analyzed directly from the raw data. At high conductances the line resistance needs to be considered and the lock-in data displayed in real units. These calculations as well as averaging over several sweeps was done with the code.

Figure 3: *Analysis**Plotting**dIdV**dIdV.py*

The **output data of the theory code** is plotted in the form of VIs and Histograms using this code:

Figure 4: *Analysis**Plotting**Theo*\ *plots_w_experimental_iqp_MT.py*

Extended Data Figure 7, 8: *Analysis**Plotting**Theo**plots_w_experimental_iqp_MT.py*

The documentation of the code for the theoretical simulations for Figure 4, Extended Data 7 and 8 is found in the end of this document.

The **topographic image** of Figure 1a) is located here:

RawData/Main/Topo/pb(111)_0029.sxm

Raw Data Assignment:

The Raw Data that are evaluated and used in the figures of the manuscript can be found here: *RawData/ …*

Main Text:

Figure 1 b)-d): *Main/VIs/*

Josephson_0_0_Cr_10mV_500nA_2000sw_1500pts_00001.dat (sweep5)
Josephson_0_0_Mn_10mV_500nA_500sw_1500pts_00001.dat (sweep5)
Josephson_0_0_Pb_10mV_500nA_2000sw_1500pts_00001.dat (sweep5)

Figure 2a: *Main/Jos_Cr/ (all files)*
Figure 2b: *Main/Jos_Mn/ (all files)*
Figure 2c: same as 2a and 2b as well as: *Main/Jos_PbrefMn/ (all files)*
Main/Jos_PbrefCr/ (all files)

Extended Data Figures:

Extended Data Figure 1:
a *Main/Jos_PbrefMn/ Jo_201126_0_0_PbCluster_500nA10mV50us1800pts500sw_comparison_ (00001…00005)*
b *Main/Jos_Cr/Jo_0_0_10mV500nA_50us1800pts2000sw_CrAtom_(00021…00040)*
c *Main/Jos_Mn/ Jo_201126_0_0_PbCluster_500nA10mV50us1800pts500sw_comparison_ (00006…00010)*

Extended Data Figure 2:
Main/Jos_PbrefCr/Jo_0_0_10mV500nA_50us2000pts2000sw_CrAtom_ (00001…00020)
Extended Data Figure 3:
Main/Jos_Cr/Jo_0_0_10mV500nA_50us1800pts2000sw_CrAtom_(00021…00040)
Extended Data Figure 4:
Main/Jos_Mn/ Jo_201126_0_0_PbCluster_500nA10mV50us1800pts500sw_comparison_ (00006…00010)
Extended Data Figure 5: *Main/Jos_Cr/ (all files)*
Main/Jos_Mn/ (all files)
Main/Jos_PbrefCr/ (all files)
Main/Jos_PbrefMn/ (all files)

Extended Data Figure 6: *Sup/JosCrAll/ (all subfolder and subfiles)*
Sup/JosMnAll/ (all subfolder and subfiles)
Sup/JosPbAll/ (all subfolder and subfiles)
Main/Jos_Cr/ (all files)
Main/Jos_Mn/ (all files)
Main/Jos_PbrefCr/ (all files)
Main/Jos_PbrefMn/ (all files)

Processed Data Assignment: *Analysis\ExtractSwitchRetrap\JosephsonSwitchRetrap.py*

As mentioned above the for figure 1 and 2 of the main text as well as for Extended Data Figures 1-6 the post processed data generated by Analysis\ExtractSwitchRetrap\JosephsonSwitchRetrap.py was used. Though the information is in the raw data as given above the processed data files can be found here: *Results/ …*

Main Text:

Figure 1: *2105_PbCr_Josephson\210623_Rdep2_MnPbCr\...*
Cr\Cr_10mV500nA2000sw\IV\...
VI_file_1_sweep_5_bwd
VI_file_1_sweep_5_fwd
Mn\Mn_10mV500nA2000sw\IV\...
VI_file_1_sweep_5_bwd
VI_file_1_sweep_5_fwd
Pb\Pb_10mV500nA2000sw\IV\...
VI_file_1_sweep_5_bwd
VI_file_1_sweep_5_fwd

Figure 2: *2011_PbMn_Josephson/201126_Rdep/Mn/*
2011_PbMn_Josephson/201126_Rdep/Pb/
2105_PbCr_Josepshon/210503_Rdep/Cr/
2105_PbCr_Josepshon/210503_Rdep/Pb/
Subfiles are sorted by setpoint current (at 10mV). Relevant files are located in each of the subfolders:
tabs/rze/(2000)/Bwd_Cor_rze_(2000).txt
tabs/rze/(2000)/Fwd_Cor_rze_(2000).txt

Extended Data Figures:

Extended Data Figure S1:

2011_PbMn_Josephson/201126_Rdep/Mn/500nA/
2105_PbCr_Josepshon/210503_Rdep/Pb/Pb_10mV500nA_2000sw/
2105_PbCr_Josepshon/210503_Rdep/Cr/Cr_10mV500nA_2000sw/

Subfiles are sorted by setpoint current (at 10mV). Relevant files are located in each of the subfolders:
tabs/rze/(2000)/Bwd_Cor_rze_(2000).txt
tabs/rze/(2000)/Fwd_Cor_rze_(2000).txt

Extended Data Figure S2:

2105_PbCr_Josepshon/210503_Rdep/Pb/ Pb_10mV500nA_2000sw/

Extended Data Figure 3:

2105_PbCr_Josepshon/210503_Rdep/Cr/ Cr_10mV500nA_2000sw/

Extended Data Figure 4:

2011_PbMn_Josephson/201126_Rdep/Mn/500nA/

Subfiles are sorted by setpoint current (at 10mV). Relevant files are located in each of the subfolders:
tabs/rze/(2000)/Bwd_Cor_rze_(2000).txt
tabs/rze/(2000)/Fwd_Cor_rze_(2000).txt

Extended Data Figure 5:

2011_PbMn_Josephson/201126_Rdep/Mn/
2011_PbMn_Josephson/201126_Rdep/Pb/
2105_PbCr_Josepshon/210503_Rdep/Cr/
2105_PbCr_Josepshon/210503_Rdep/Pb/

Subfiles are sorted by setpoint current (at 10mV). Relevant files are located in each of the subfolders:

tabs/rze/(2000)/Bwd_Cor_rze_(2000).txt
tabs/rze/(2000)/Fwd_Cor_rze_(2000).txt

Extended Data Figure 6: **All** Subfolders with
tabs/rze/(2000)/Bwd_Cor_rze_(2000).txt
tabs/rze/(2000)/Fwd_Cor_rze_(2000).txt

Users Guide to Python Code:

The analysis was done in Python. We provide the virtual environment for the packages which we used at the time the code was written (2019-2022, Analysis/virtEnv). The data is measured in the Franke group at Freie Universität Berlin at a low temperature Createc STM including a 1K stage. A dedicated resistor-amplifier setup was used during measurement to carry out current-biased Josephson measurements. All experimental details are given in the Methods section of the publication. Here, we provide more details on how to read and process the original data using a self-written Python code.

Analysis with *Analysis\ExtractSwitchRetrap**JosephsonSwitchRetrap.py:***

The raw data is read in and I_{sw} and I_{re} are extracted by the peaks in derivative of the IV curves. The data is smoothed by a gaussian procedure to ensure the sharpness of the peaks in the derivatives. The slope around zero (called R_0 in the code, later G_{PD}) is saved as well as the resistance after the jump to the resistive state. The amplifier gives a slowly changing offset in the measured voltage which is corrected by the zero crossing of these fits. Results are saved as .txt files containing the single IVs with a header providing the I_{re}, I_{sw} and G_{PD} (as R_0). In addition, I_{re}, I_{sw} and G_{PD} of all sweeps are summarized in a .txt files. To correct for a bias offset the mean offset in the Pb data is extracted and applied to the data on magnetic atoms. There are other corrections implemented to correct for drift in different ways but those were not used for this manuscript. The corrected data will be saved in subfolders, according to the correction s that were applied. The name is a series of numbers that indicates the kind of correction that was applied (in this case (2000), as identifier for the applied data treatments as described in the code).

Histograms will be plotted and saved for the raw as well as for the corrected data and exemplary VIs are plotted. To ensure the proper working of the applied corrections additional figures are saved, for example the evolution of I_{sw}, I_{re} and G_{PD} over time before and after the corrections are applied to account for piezo creep. In addition, a summary of the data including the extracted average values of I_{re}, I_{sw} and G_{PD} is saved. Details of the measurement parameters (date of measurement, integration time, number of points etc.) together with the settings of the python code (e.g., which corrections where used, how was the data filtered …) is save here.

For using the program, the **CONSTANTS.py** is the most important part to be adjusted before running the program. Here all the analysis details are provided. In **CONSTANTS.py** data files are loaded for the individual experiments indicating the path of the raw data files and the directories the results should be saved to. These data files are organized in subfolders within the Experiments folder in the working directory. These files need to be adjusted as well. Some more information such as measurement series, adsorption site and material are to be given as a python list which has the same length as the input files. More details are given in the comments of the code. Please ensure that the *filepaths* and *savepaths* are correct before running the code if the working directory is not the same as the directory of the executable. The code will run through all indicated files. Parallelization is used if the right number of processors is given in the **CONSTANTS.py** file.

IMPORTANT: *For correcting the bias offset the mean bias offset of the Pb-Pb junction is used from the summary file which is saved for each series and applied to the magnetic atom junction of the same series. For that reason, it is important that the Pb data already exists for the measurement series when running it for the magnetic atoms****. It is important to run the Josephson data on Pb before any measurements on magnetic atoms and indicate the same measurement series****. Otherwise, the data cannot be found and used to correct the offset on any other atom.*

The run file of the code is called **JosephsonSwitchRetrap.py.** If all data in **CONSTANTS.py** is correct the code does not need any adjustments to provide the data.

To reproduce the data the **CONSTANTS.py** file only needs minor adjustments to run with the data that is used in the manuscript. Please make sure the correct numbers of processors is entered. Also note that the amplifier gain changes for one set of measurement to the other and needs to be adjusted as explained in the comments of the code. The most important changes are to be made in the individual data files for the measurement times. Make sure that the right paths to the data that you want to analyze is entered. As presented here they will lead to the right directory as long as the working directory is set to be in the same folder as **JosephsonSwitchRetrap.py** and all folders from the Refubium are saved in a folder called **DataAnalysis** and the subfolders indicated in the beginning of this document.

For example the raw data is located at:
'V:/Papers/22-01-Josephson-diode/DataAnalysis/RawData/Main/Jos_Cr'
The path is given with:
'../../DataAnalysis/RawData/Main/Jos_Cr'

which indicates the location within the **DataAnalysis** folder. However, depending on the system you might need to put in the full path as it is on your computer.

The same holds true for the safe path location. Please enter here where you would like to save all the results from the code. It might be quite a large amount of data. The directories will be created automatically.

Further analysis: *Analysis/Plotting/*

There are several python codes that are used to plot the data coming from the previously described code. The paths in these scripts lead to the right directory if the working directory is set to the '*Plotting*' folder which is generally located two instances above the folder that contains the code. If the working directory is not the same, the directories of the resulting switching and retrapping currents as provided by **JosephsonSwitchRetrap.py** need to be selected for *Filepath*. If the resulting images should be saved, an existing directory path needs to be entered in the variable *Savepath*. As presented here, the images

will be shown as output of the code but will not be saved. More details are given in the comments of the code directly.

IswIre_GPD .py: Figure 2, Extended Data Figure 5, 6

The extracted switching and retrapping currents from **JosephsonSwitchRetrap.py** are used. We average the data in sets of one hundred points, to account for piezo creep which changes the junction conductance. For some of the individual IVs of extracted data at low conductance switching and retrapping currents may be assigned the wrong way. If that is the case the code corrects for it by checking each file for the wrong signs. Subsequently the data is plotted in several different ways.

dIdV.py: Figure 3 a-d, f

For the voltage bias data, the series resistance of the lines needs to be accounted for at higher conductance. This is done here providing the knowledge about the coherence peak energy of Pb. Regauging is also done here. It plots directly from the Raw data as measured by the STM.

Histo_plot.py: Extended Data Figure 1, 2, 3, 4

The extracted switching and retrapping currents from **JosephsonSwitchRetrap.py** are used to plot histograms from it. It also provides several histograms for sets of 100 sweeps to visualize the issue of creep.

plots_w_experimental_iqp_MT.py: Figure 4, Extended Data 7, 8, 9

Plots Histograms and VIs from the output data of the theoretical simulation code.

VI.py: Figure 1 a-d

Plots single VIs from the data saved by **JosephsonSwitchRetrap.py** where the switching and retrapping currents as well as GPD are saved in the header of each individual VI.

Theoretical simulations: *TheoSim*\

The directory contains two folders: *TheoSim**library*\ contains the Python script containing the Euler-Maruyama algorithm. *TheoSim**retrapping_and_switching_currents**experimental_data*\ contains the experimental current measurements used in the theoretical simulations as well as the Python script for extracting the quasiparticle current. This is called by the scripts *TheoSim**retrapping_and_switching_currents**RCSJ_experimental_data_XYZ.py* (XYZ = Kauz_Martinis, mn_symmetric_noise_Kauz_Martinis, pb_and_asym_Ic_Kauz_Martinis) which run the simulations used in Figure 4 and Extended Data Figures 7 and 8. Finally, *TheoSim**retrapping_and_switching_currents**plots_w_experimental_iqp.py* extracts the switching and retrapping currents and plots the data.