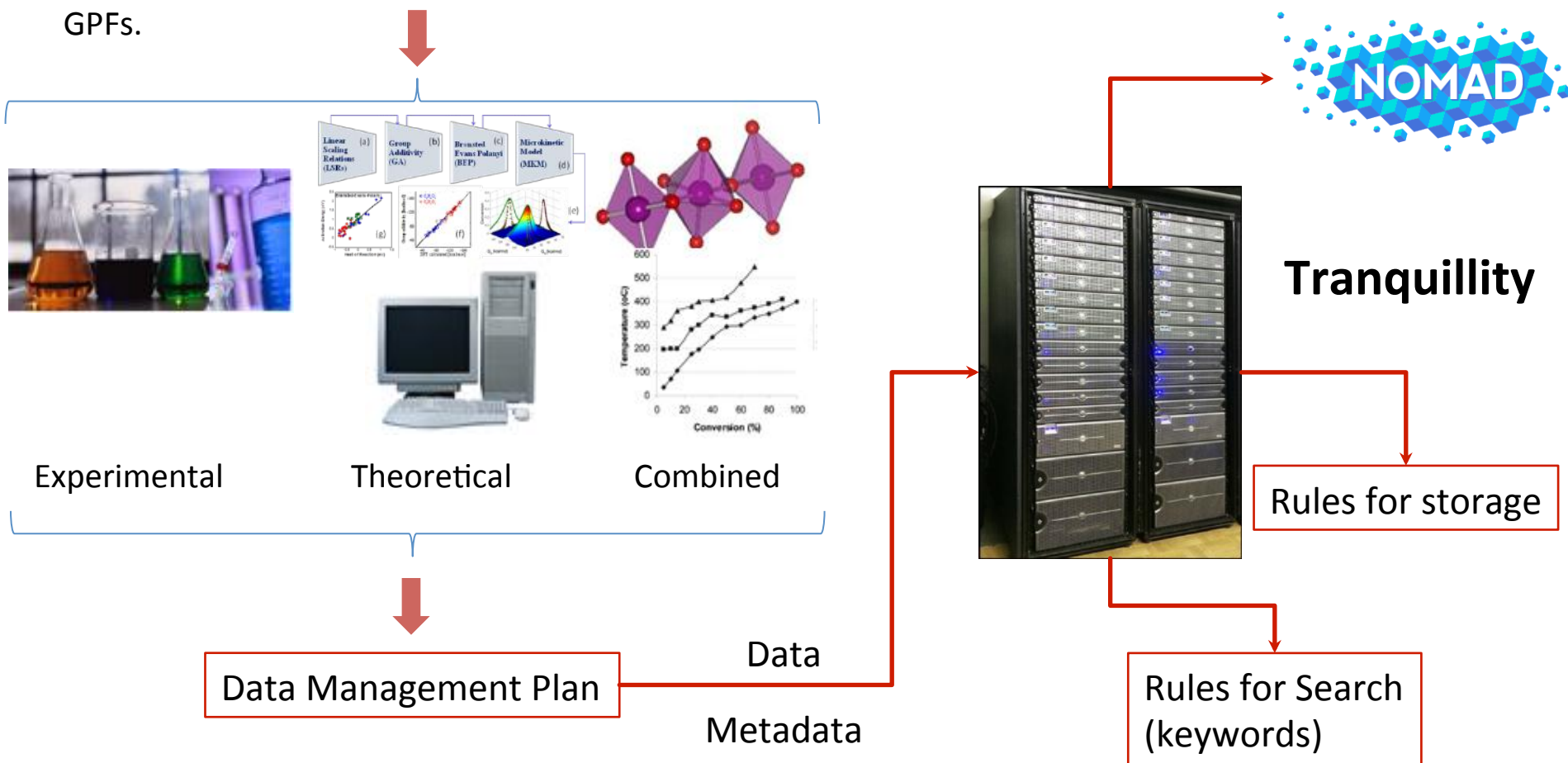


**“Development of novel, high Performance
hybrid TWC/GPFs Automotive after treatment
systems by rational design: substitution of
PGMs and Rare earth materials”
PARTIAL-PGMs”**

Experience on Experimental Metadata

PARTIAL-PGMs Approach

PARTIAL-PGMs proposes an integrated approach for the coherent development of smart and innovative nanostructured automotive post-treatment systems by **integrating TWCs on GPF**, capable to meet future regulations, with **reduced CRMs**, leading to development of 2nd generation GPFs.



Experimental Metadata

Experimental Template Documents

Adsorption isotherms

TPR

UV-Vis spectroscopy

Adsorption isotherm:

Type:	<i>#Experimental, ab initio, DFT</i>	(STR)
Adsorbate:	<i>#Name of the adsorbate</i>	(STR)
Temperature:	<i>#Temperature used</i>	(FLOAT)
Pressure range:	<i>#Pressure range of the isotherm</i>	(FLOAT – FLOAT)
Outgassing temperature:	<i>#Temperature used fro outgassing</i>	(FLOAT)
Sample weight:	<i>#Mass of the sample used</i>	(FLOAT)
BET value:	<i>#value of the surface area</i>	(FLOAT)
Total pore volume:	<i>#pore volume of the sample</i>	(FLOAT)

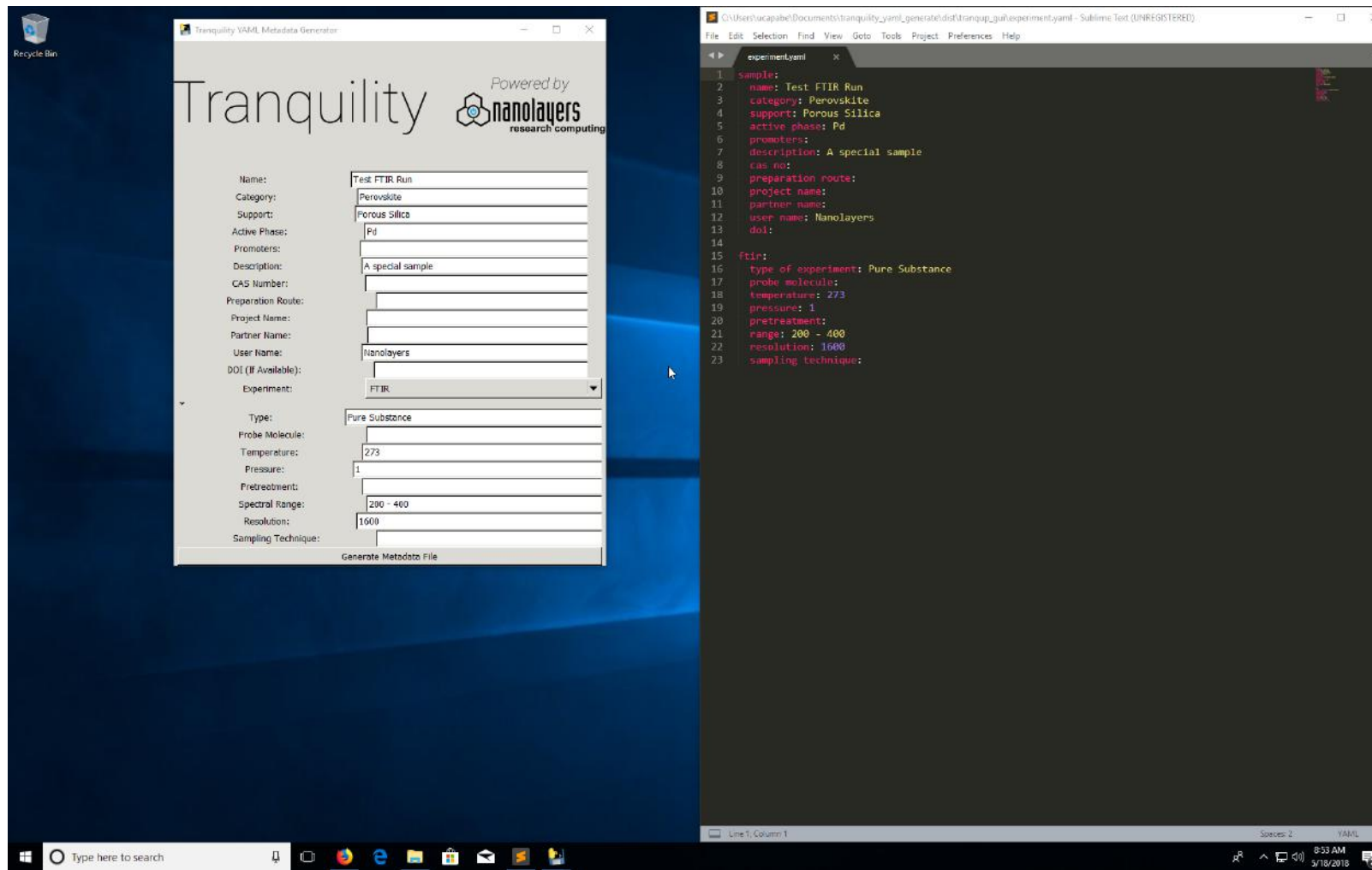
UV/Vis:

Range:	<i>#Spectral range</i>	(FLOAT – FLOAT)
Pre-treatment:	<i>#Pre-treatment conditions if applicable</i>	(STR)
Sampling Technique:	<i>#Diffuse reflectance or other</i>	(STR)

TPR:

Type of the experiment :	<i>#Flow or Pulse</i>	(STR)
Probe molecule:	<i>#1 night at 1E-5 mbar</i>	(STR)
Pretreatment:	<i>#Gas type, flow and temperature range</i>	(STR)
Temperature range:	<i>#Temperature used</i>	(FLOAT – FLOAT)
Temperature increase rate:	<i>#Rate of temperature increase</i>	(FLOAT)
Flow conditions:	<i>#Flow of the gas</i>	(FLOAT)

YAML File for FTIR



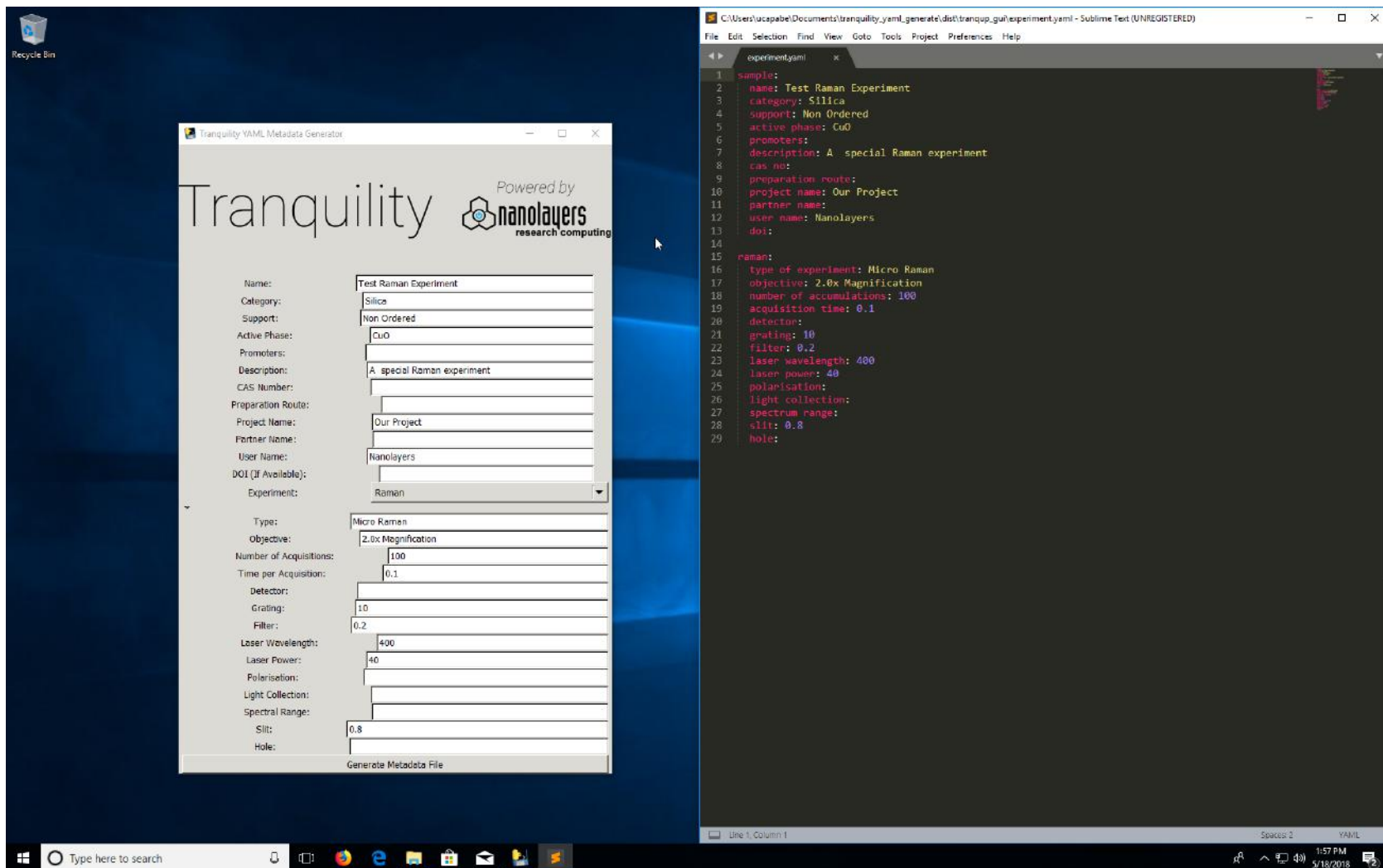
The image shows a Windows desktop environment. On the left, the 'Tranquility' GUI is open, displaying a form for generating a metadata file. The form fields are filled with the following information:

- Name: Test FTIR Run
- Category: Perovskite
- Support: Porous Silica
- Active Phase: Pd
- Promoters:
- Description: A special sample
- CAS Number:
- Preparation Route:
- Project Name:
- Partner Name:
- User Name: nanolayers
- DOI (If Available):
- Experiment: FTIR
- Type: Pure Substance
- Probe Molecule:
- Temperature: 273
- Pressure: 1
- Pretreatment:
- Spectral Range: 200 - 400
- Resolution: 1600
- Sampling Technique:

At the bottom of the GUI, there is a 'Generate Metadata File' button. On the right, a Sublime Text editor window is open, displaying the generated YAML file 'experiment.yaml'. The content of the file is as follows:

```
1 sample:
2   name: Test FTIR Run
3   category: Perovskite
4   support: Porous Silica
5   active phase: Pd
6   promoters:
7   description: A special sample
8   cas no:
9   preparation route:
10  project name:
11  partner name:
12  user name: Nanolayers
13  doi:
14
15  ftir:
16    type of experiment: Pure Substance
17    probe molecule:
18    temperature: 273
19    pressure: 1
20    pretreatment:
21    range: 200 - 400
22    resolution: 1600
23    sampling technique:
```

YAML File for Raman



The image shows a Windows desktop environment. On the left, the 'Tranquility YAML Metadata Generator' application is open. It features a form with various fields for entering experiment details. The 'Name' field is filled with 'Test Raman Experiment'. Other fields include 'Category: Silica', 'Support: Non Ordered', 'Active Phase: CuO', 'Description: A special Raman experiment', 'Project Name: Our Project', 'Partner Name: Nanolayers', 'User Name: Nanolayers', 'Experiment: Raman', 'Type: Micro Raman', 'Objective: 2.0x Magnification', 'Number of Acquisitions: 100', 'Time per Acquisition: 0.1', 'Detector', 'Grating: 10', 'Filter: 0.2', 'Laser Wavelength: 400', 'Laser Power: 40', 'Polarisation', 'Light Collection', 'Spectral Range', 'Slit: 0.8', and 'Hole'. A 'Generate Metadata File' button is at the bottom.

On the right, a Sublime Text editor window titled 'experiment.yaml' displays the following YAML code:

```
1 sample:
2   name: Test Raman Experiment
3   category: Silica
4   support: Non Ordered
5   active phase: CuO
6   promoters:
7   description: A special Raman experiment
8   cas no:
9   preparation route:
10  project name: Our Project
11  partner name:
12  user name: Nanolayers
13  doi:
14
15 raman:
16  type of experiment: Micro Raman
17  objective: 2.0x Magnification
18  number of accumulations: 100
19  acquisition time: 0.1
20  detector:
21  grating: 10
22  filter: 0.2
23  laser wavelength: 400
24  laser power: 40
25  polarisation:
26  light collection:
27  spectrum range:
28  slit: 0.8
29  hole:
```