Supporting Information

for

PANDA: A self-driving lab for studying electrodeposited polymer films

Harley Quinn,[a] Gregory A. Robben,[a] Zhaoyi Zheng,[a] Alan L. Gardner,[b] Jörg G. Werner,*[abc] and Keith A. Brown*[abd]

[a]Division of Materials Science & Engineering, Boston University, Boston, MA, 02215, USA.

[b]Department of Mechanical Engineering, Boston University, Boston, MA, 02215, USA

[c]Department of Chemistry, Boston University, Boston, MA, 02215, USA

[d]Department of Physics, Boston University, Boston, MA, 02215, USA

*E-mail: brownka@bu.edu, jgwerner@bu.edu

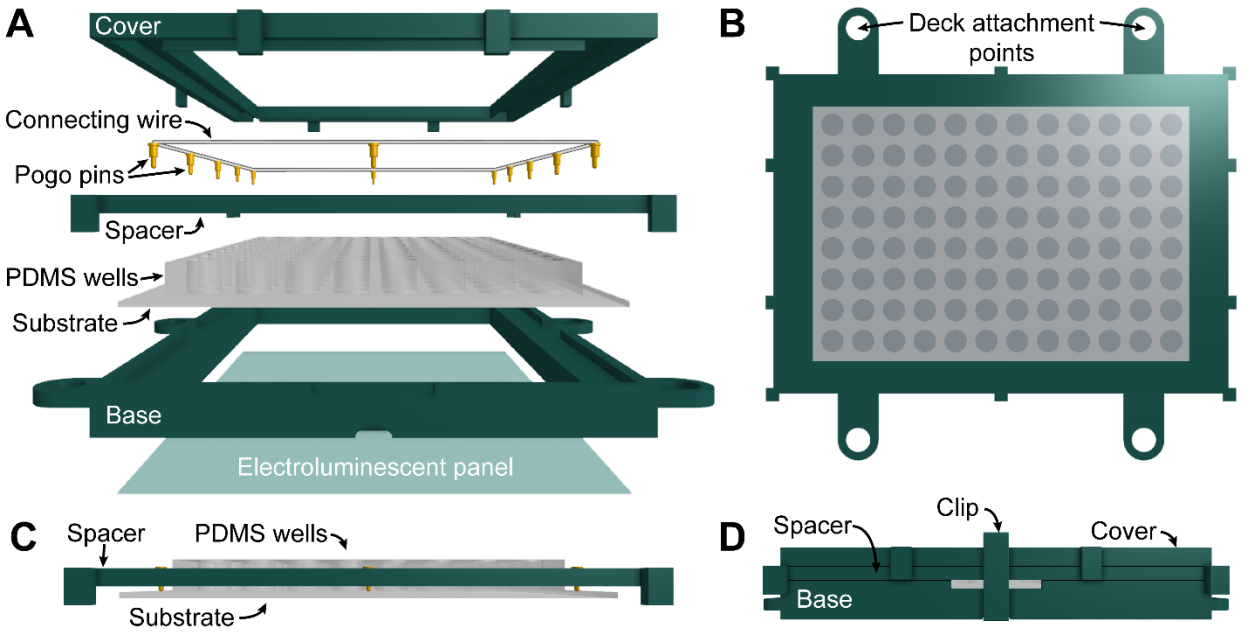

Fig. S1 (A) Exploded view of substrate holder including the electroluminescent panel (27260-P, TechnoLight) used for optical transmission measurements. (B) Top view of holder with polydimethylsiloxane (PDMS) wells on substrate illustrating screw holes where it attaches to the deck. (C) Front view of substrate with PDMS wells showing the spacer and how gold-coated pogo (spring-loaded) pins contact the conductive surface of the transparent substrate. (D) Front view of fully assembled substrate holder with clip holding pieces together.

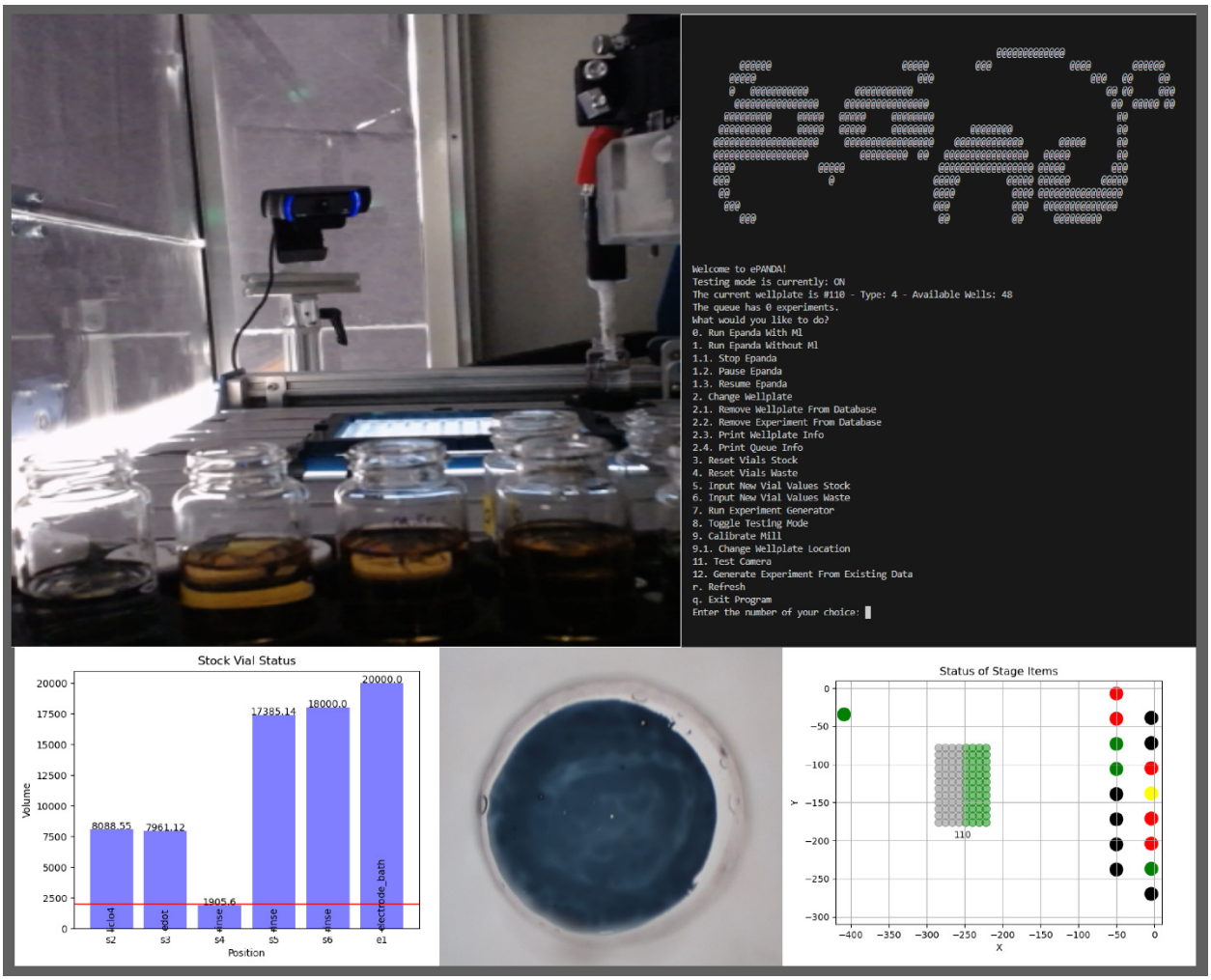

Fig. S2 Full resolution version of Figure 1C.

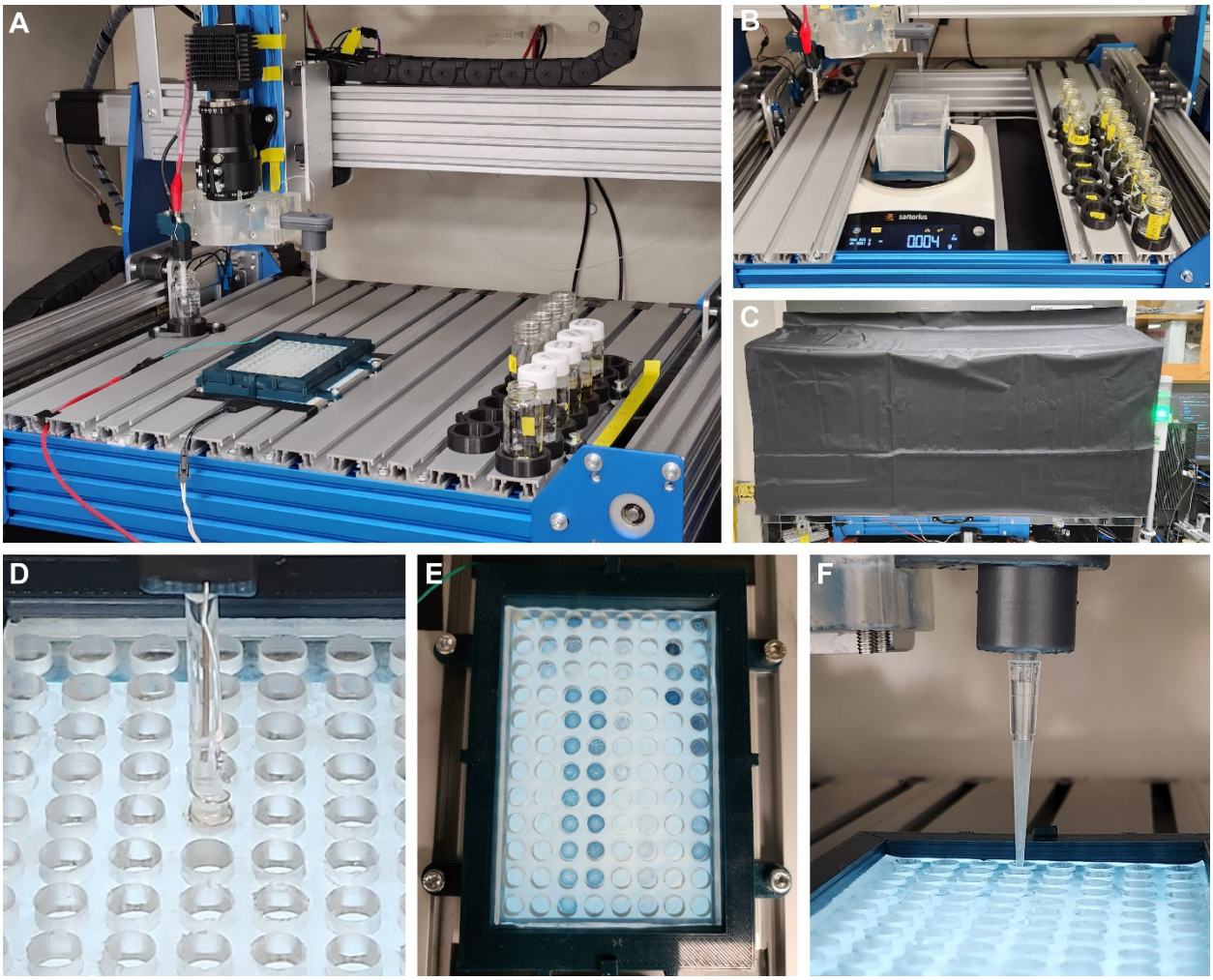

Fig. S3 (A) Picture of the PANDA instrument deck with the reference electrode in electrolyte solution. (B) View of the PANDA deck with a panel removed for the scale, used in the liquid handling validation experiments. (C) PANDA enclosure with light blocking curtain installed for electrochromic experiments. (D) Close up view of counter and reference electrode in one of the PDMS wells. (E) Top view of the PDMS well plate over the electroluminescent panel with PEDOT:PSS films electrodeposited in some of the wells. (F) Close up view of the liquid handling system's pipette tip, removing solution from one of the wells after an experiment.

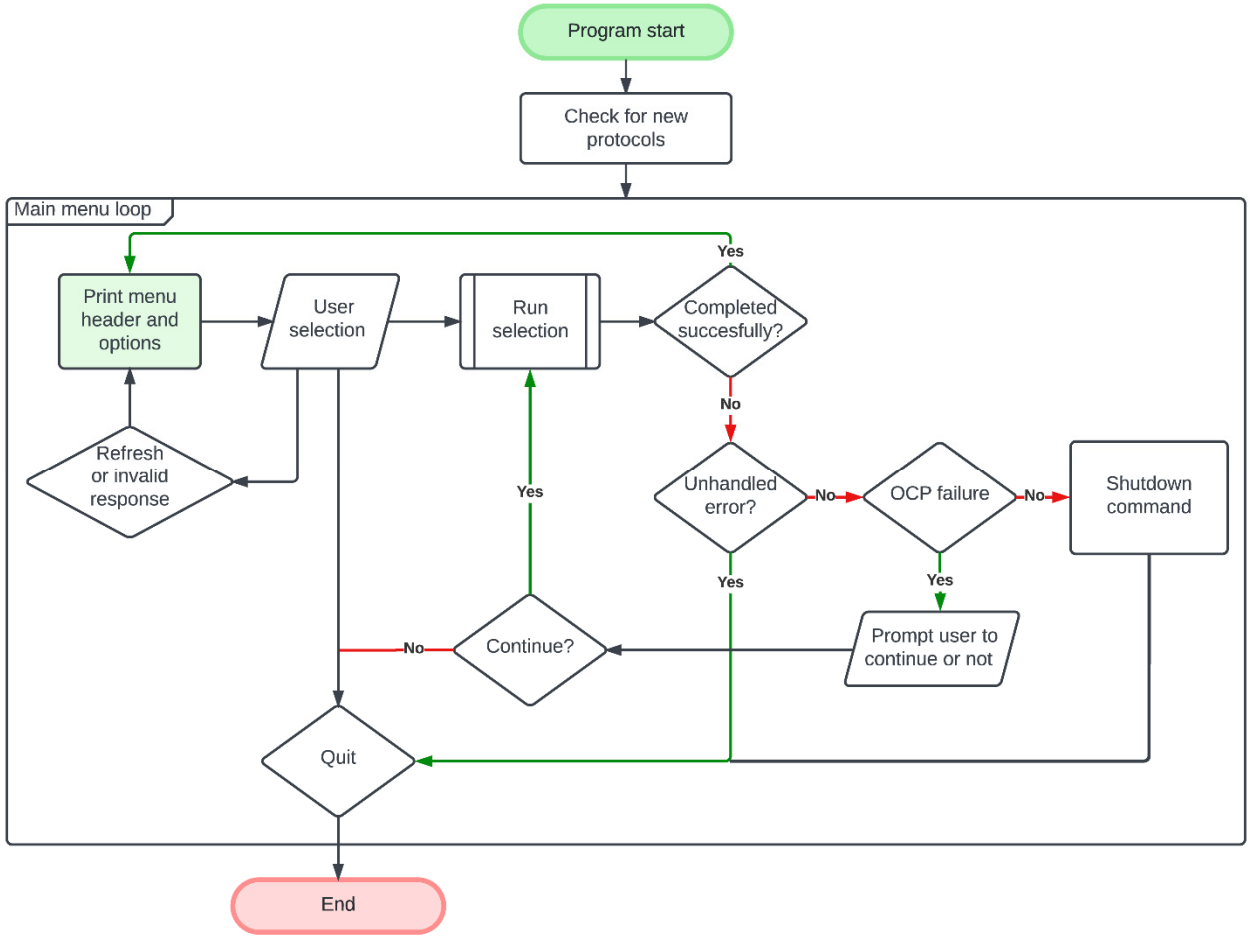

Fig. S4 Flowchart of PANDA software main menu.

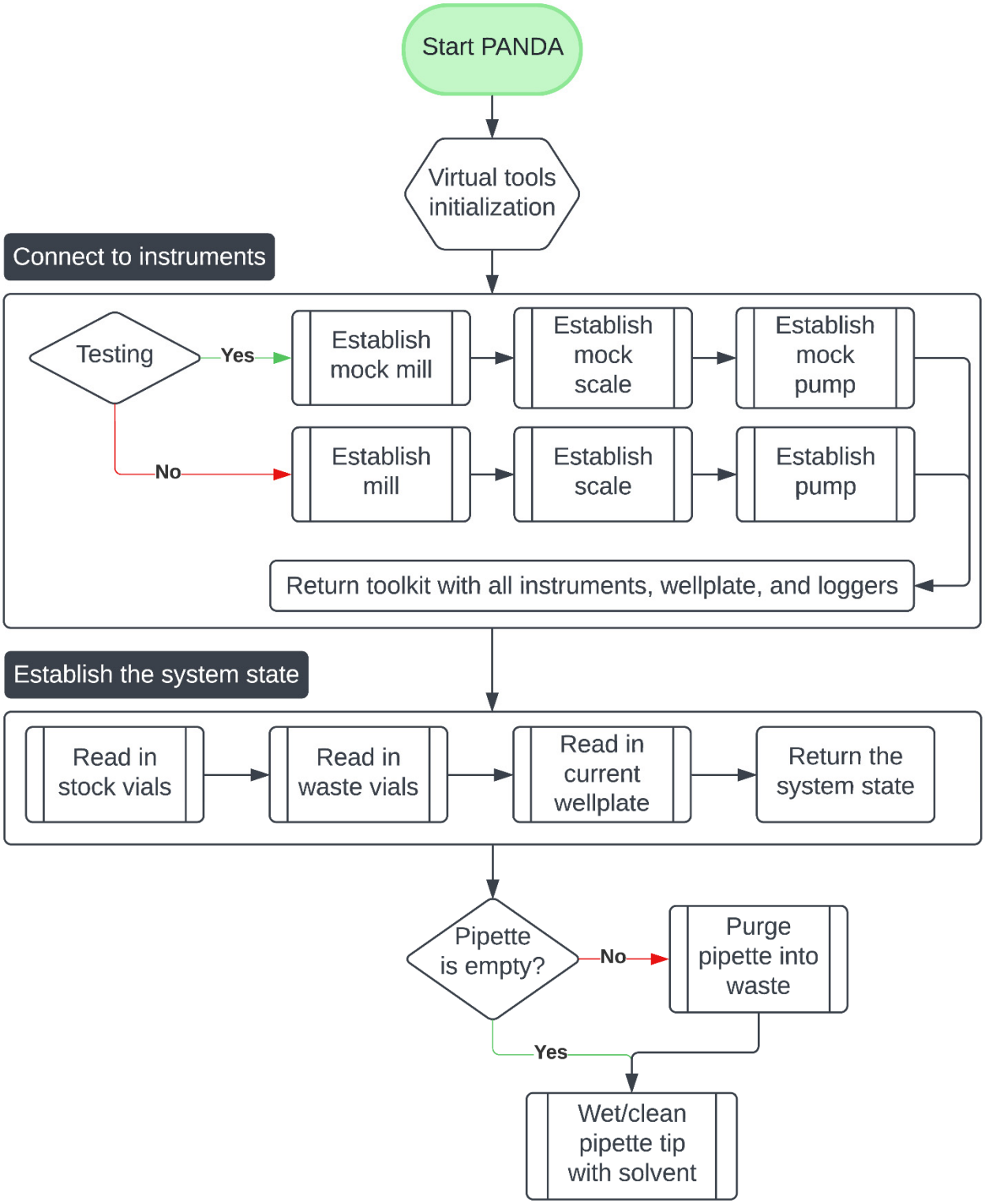

Fig. S5 Flow chart showing initialization of PANDA prior to running the experiment loop.

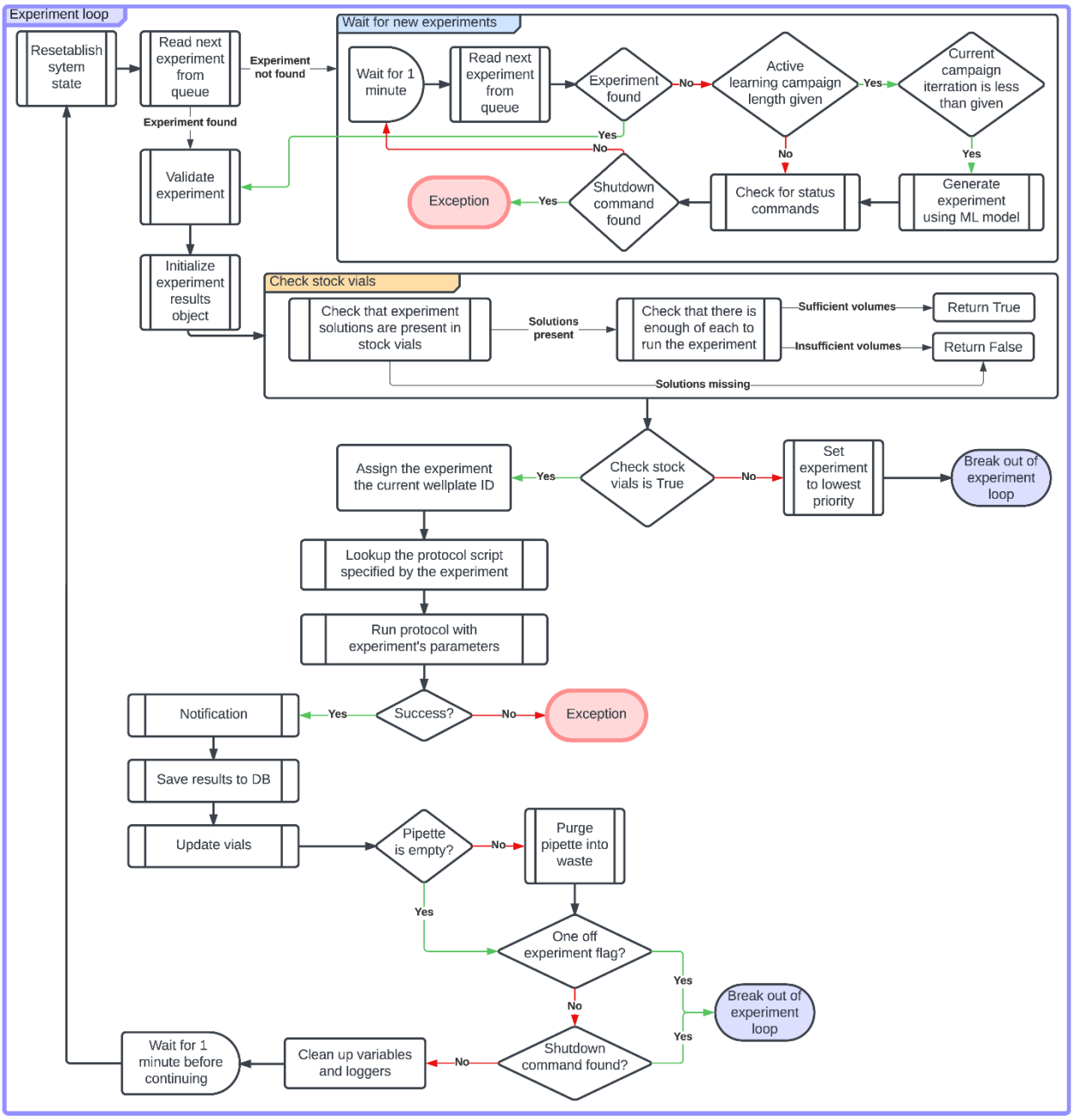

Fig. S6 Flowchart of PANDA software showing experiment loop.

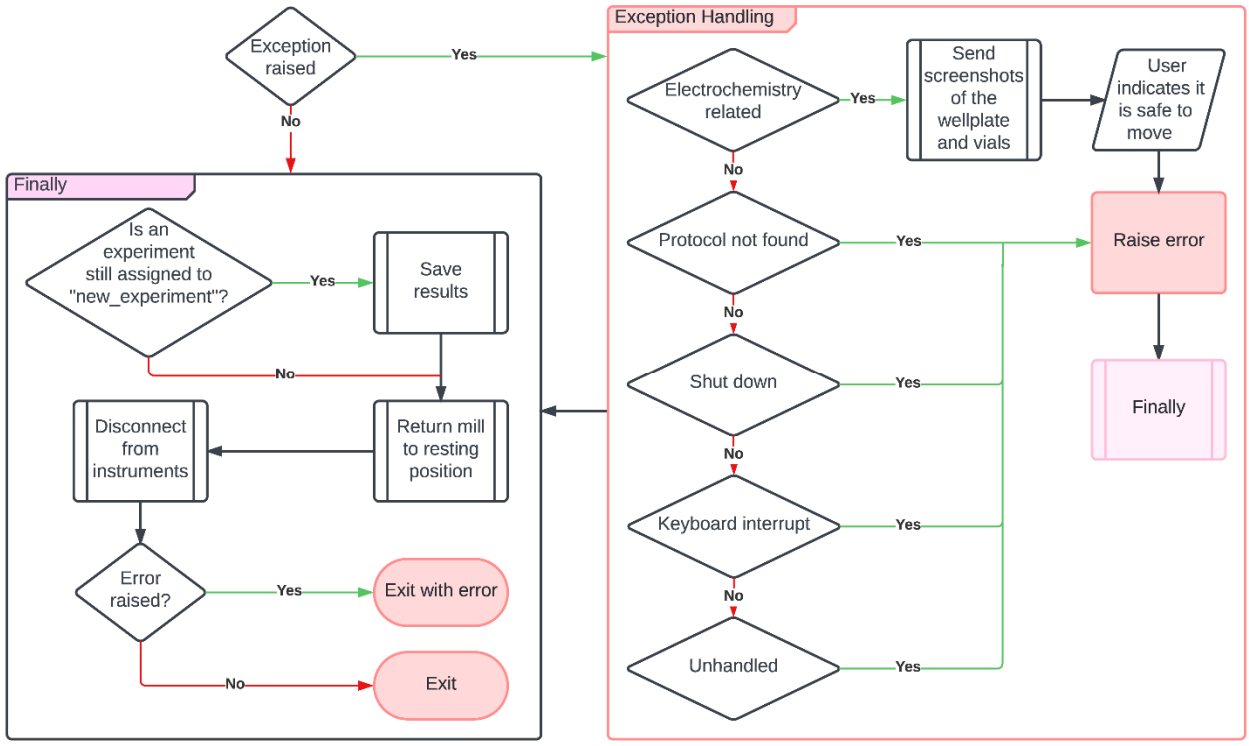

Fig. S7 Flowchart of PANDA software demonstrating the end of the experiment loop, with error handling and shutting down the PANDA.

Table S1 Open-source Python (version 3.11.9) packages used by the PANDA

Purpose	Package Name	Version	Source
Cameras	obsws-python	1.7.0	https://pypi.org/project/obsws-python/
Machine Learning	gpytorch	1.11	https://pypi.org/project/gpytorch/
Data visualization	matplotlib	3.8.4	https://pypi.org/project/matplotlib/
Data handling	pandas	2.2.2	conda-defaults
Liquid handling calculations	pulp	2.8.0	conda-forge
Data validation	pydantic	2.5.3	conda-defaults
Instrument communication	pyserial	3.5	conda-defaults
Slack communications	regex	2023.10.3	conda-defaults
Image processing	scikit-image	0.23.2	conda-defaults
Machine learning	scikit-learn	1.4.2	conda-defaults
Slack communications	slack-sdk	3.19.5	conda-defaults

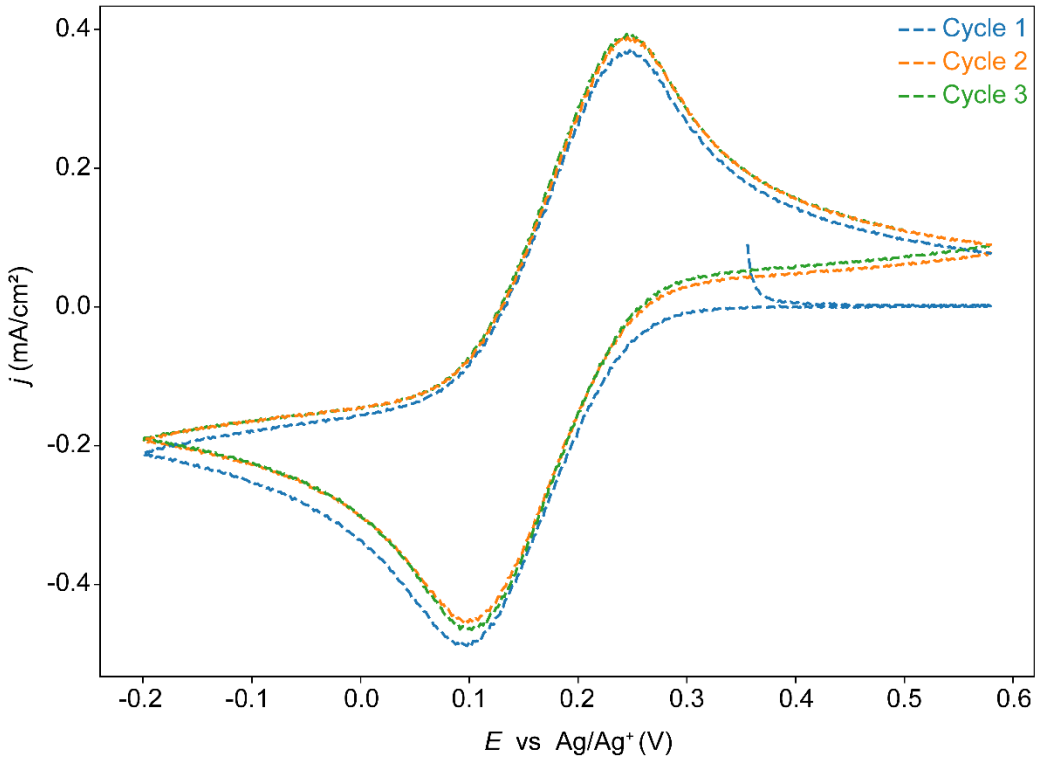

Fig. S8 Example of a cyclic voltammogram of the $K_3Fe(CN)_6$ experiment showing three cycles. Cycle 2 is used for all analyses.

Table S2 Potentiostat settings for cyclic voltammetry experiments

Relevant Figure	Scan rate (mV/s)	Step size (mV)	Scan limit 1 (V)	Scan limit 2 (V)
3B, 3C	50	2	-0.2 vs Ag/Ag+	0.58 vs Ag/Ag+
3D	50	2	-0.2 vs Ag/Ag+	0.58 vs Ag/Ag+
3F	50	2	-0.2 vs Ag/Ag+	0.58 vs Ag/Ag+

Table S3 Potentiostat settings for chronoamperometry experiments

Relevant Figure	Purpose	Potential applied (V)	Time potential applied (s)
5A	Film deposition	1.26 vs Ag/Ag^+	4.2
5A	Film reduction	-0.6 vs Ag/Ag^+	60
5B	Film deposition	0.8 – 1.6 vs Ag/Ag^+	1 – 100
5B	Film reduction	-0.6 vs Ag/Ag^+	60

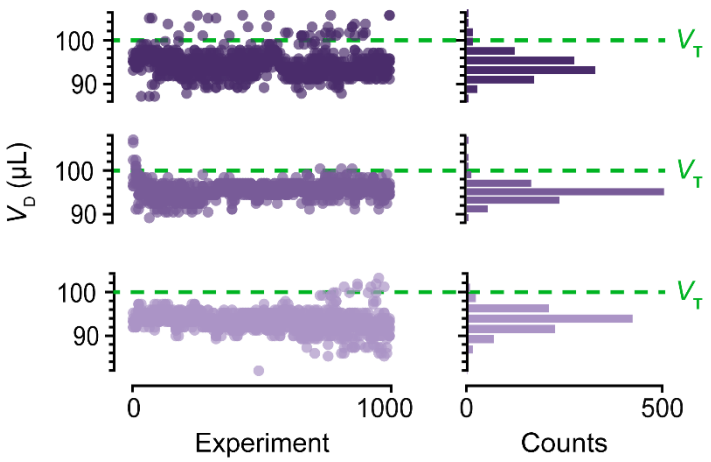

Fig. S9 Plot showing three different pipette tips each performing 1000 fluid deposition experiments using forward pipetting, plotting experiment volume dispensed V_D vs. experiment number. Histograms show the frequency of dispensed volumes. The target volume V_T of 100 µL is marked by a dashed green line. RMSE for each pipette tip from top to bottom, 2.8 µL, 1.8 µL, and 2.2 µL.

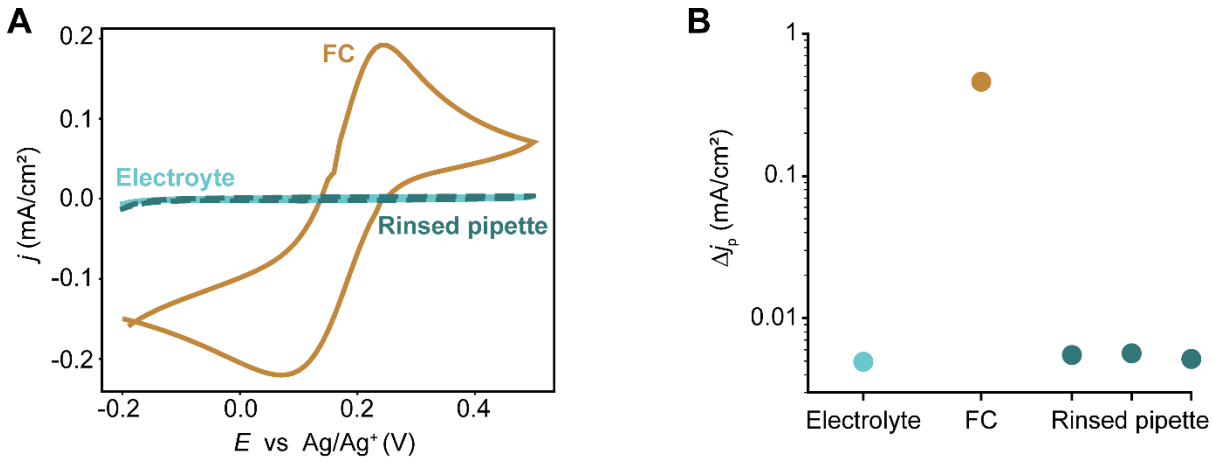

Fig. S10 (A) Cyclic voltammograms (CVs) of an electrolyte solution (light teal), ferricyanide solution (FC), and electrolyte solution dispensed with a rinsed pipette (dark teal) performed with operating voltage between -0.2 and 0.5 V, scan rate 50 mV s^{-1}. (B) Plot showing the peak-to-peak current density Δj_p values obtained for each CV from A.

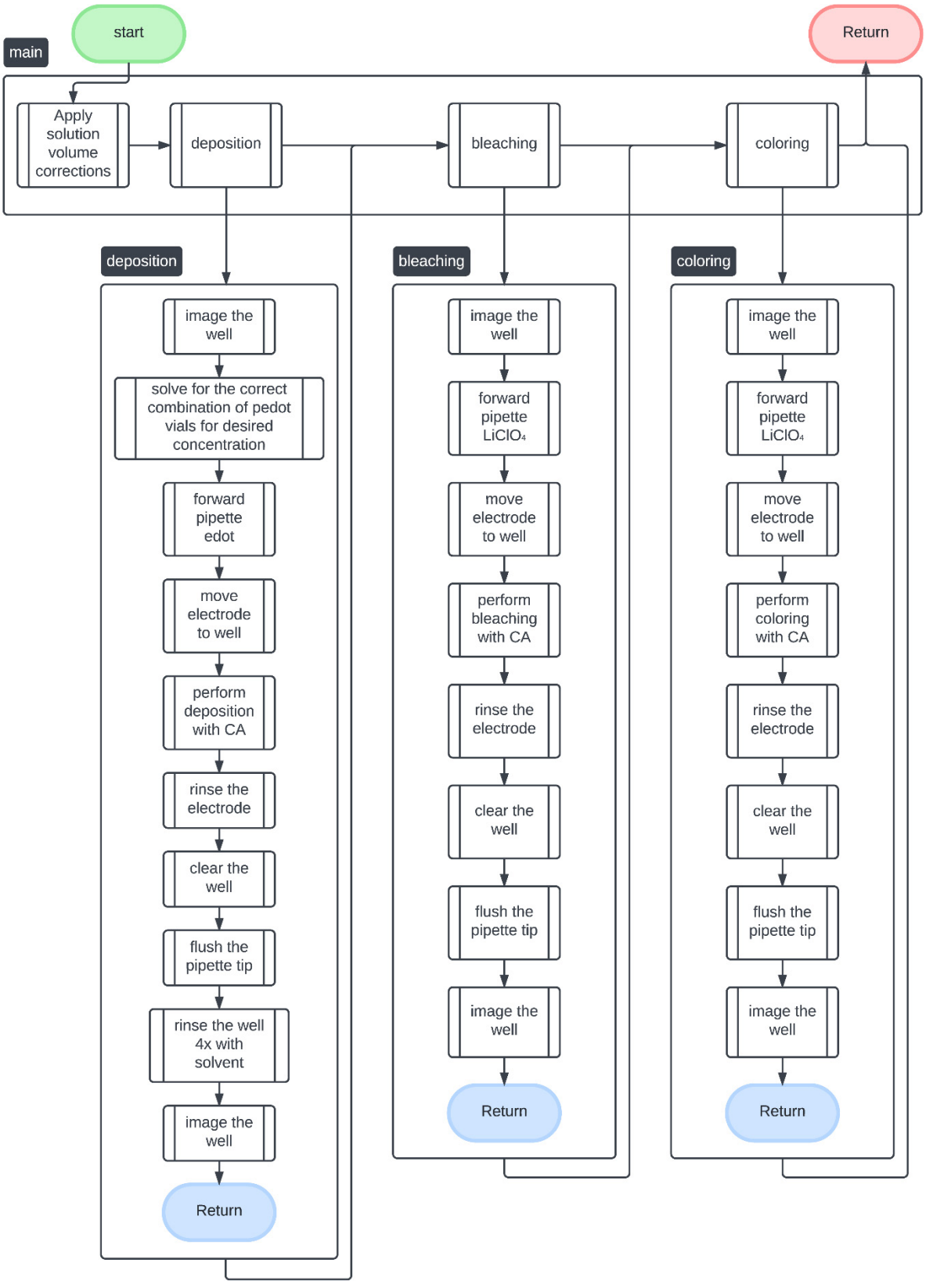

Fig. S11 Flowchart illustrating the protocol for PEDOT:PSS experiments.