Project 2.1 Towards Organic Protonic Memristors

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WWW: https://www.icho.edu.pl/en/zespol/cina-foroutan-nejad-research/

Background: Computational Chemistry

Aim:
This interdisciplinary project aims to develop next-generation molecular electronic devices that combine **information storage and processing at the molecular scale**. The research integrates **computational modeling, organic synthesis, and device characterization**, with strong national and international collaboration (including CeNT at the University of Warsaw and Kavli Institute of Nanoscience at TU Delft). The computational component plays a central role in:

- Designing molecules with **efficient proton-transfer switching**
- Predicting **conductance properties and on/off ratios**
- Guiding experimental synthesis and device fabrication

The work combines **density functional theory (DFT)** and **nonequilibrium Green's function (NEGF)** methodologies to model charge transport and switching phenomena

Scope of Work
The successful candidate will:

- Perform **first-principles simulations (DFT)** of molecular systems
- Investigate **proton transfer mechanisms under external electric fields**
- Analyze **energy barriers and switching pathways**
- Study **structure–property relationships** in memristive molecules
- Collaborate closely with experimental teams to guide synthesis
- Contribute to **scientific publications and conference presentations**

The PhD student will focus specifically on the **computational design and analysis of organic molecules for memristive devices**.

Requirements:
Applicants should:

- Hold a **Master's degree** in chemistry, physics, materials science, or a related field
- Have a solid background in **computational chemistry**
- Be familiar with **DFT methods and electronic structure theory**
- Have experience with software such as *Gaussian, ORCA, SIESTA*, or similar
- Possess strong analytical and problem-solving skills
- Be able to work both **independently and in a multidisciplinary team**
- Have good command of **English (written and spoken)**

Additional assets:

- Experience with **programming/scripting (Python, Bash)**
- Interest in **molecular electronics or materials science**