Computational screening of organic molecules for flow battery applications

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compbat

https://compbat.eu/

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State of the art: RFBs

1 MW, 5 h

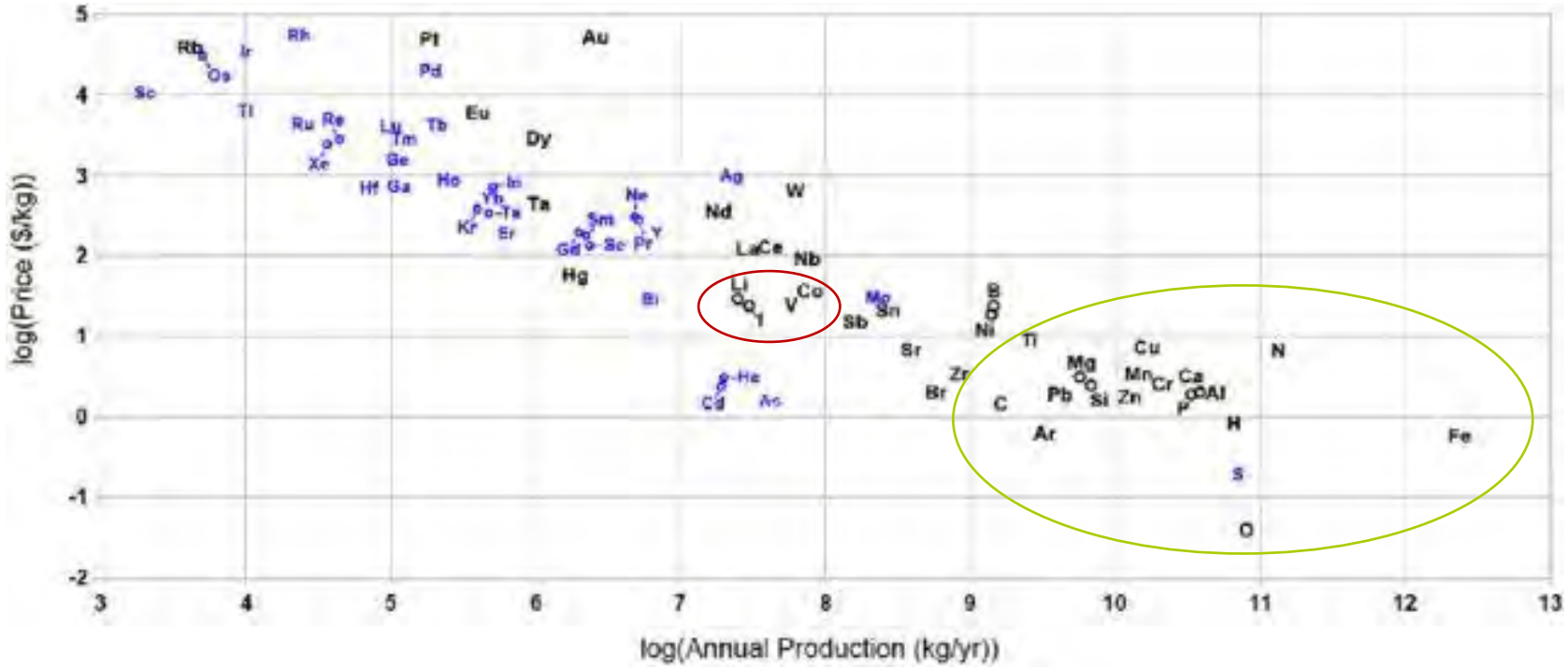
State of the art: RFBs

Too expensive, not enough V production

1 M[illegible], 5 h

What alternatives?

What elements?



Fe, Cr, Al, Mn, Cu, Ti

Organic compounds

Vesborg & Jaramillo, RSC Advances, 2012, 2, 7933-7947

What alternatives?

- Organic molecules
  - Pontentially inexpensive
  - Performance in pair with VRFBs
  - Sustainable?
- Metal complexes
  - Fe, Ti, Mn and other metals available in large scale
  - New ligands required
- Questions
  - Synthesis?
  - Stability?
  - Cost?

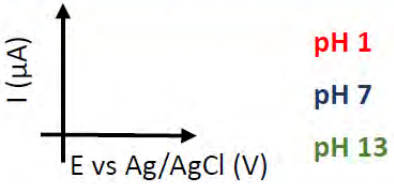
Tunable by changing structure

How to choose the materials?

Experimental approach

- Test everything that could be redox active that we have in the cupboards
  - We even found some chemicals made in Germany in 1930-1940s.
  - Tested >20 compounds

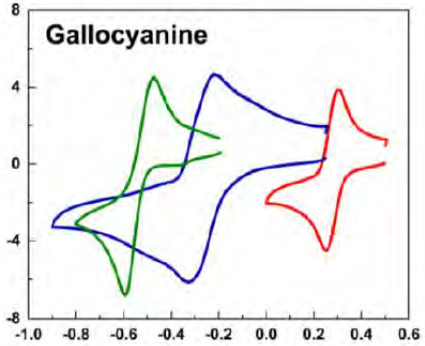
Results

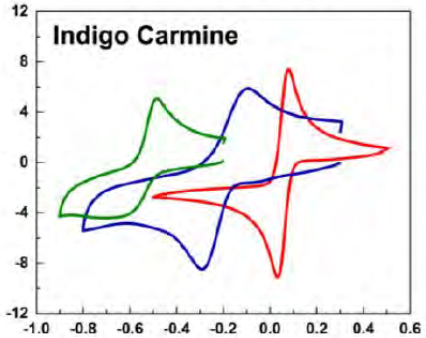


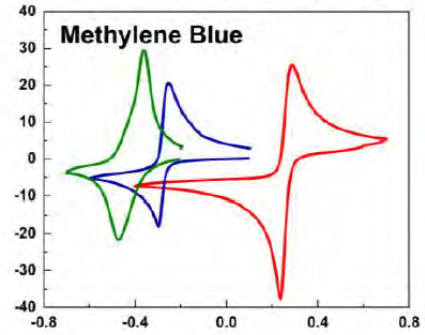
pH 1

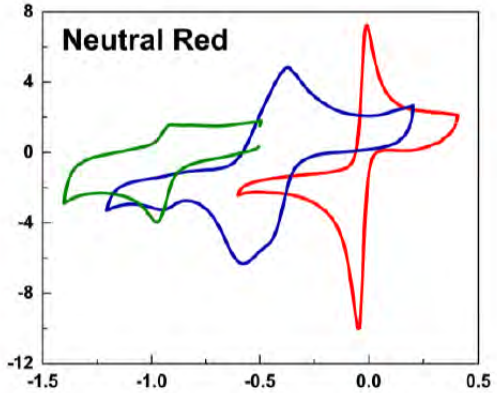
pH 7

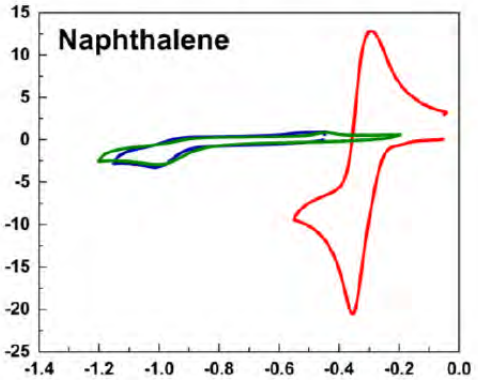
pH 13

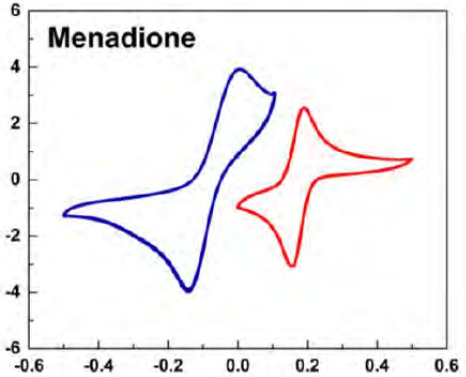


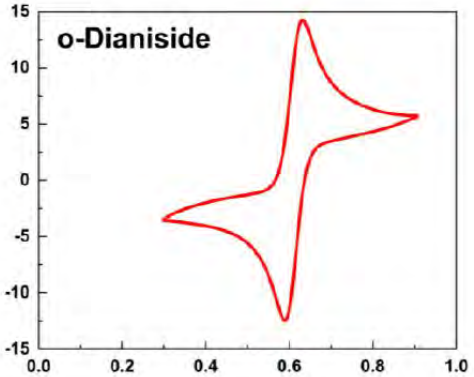


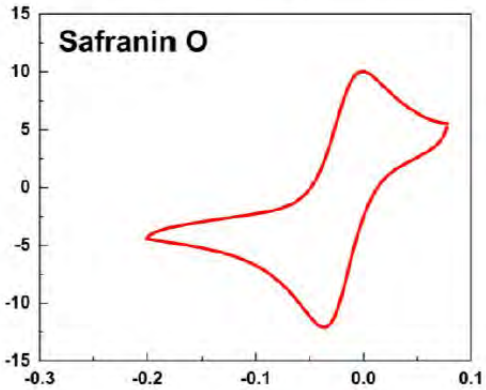


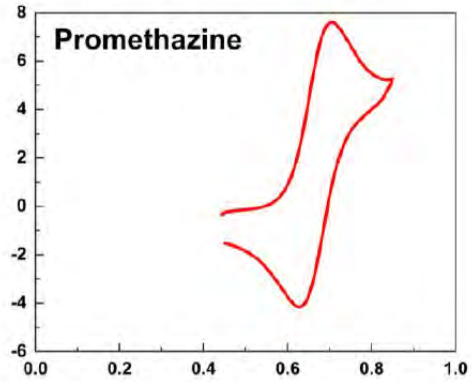












Rasmus Rönkä,
Mahsa Shahsavan

Computer aided screening of materials

- Advanced computational tools
  - Density functional theory
    - Build up a database
  - Machine learning
    - Understanding of trends

  - Evaluation of redox potentials and solvation free energies