UCDAVIS
UNIVERSITY OF CALIFORNIA

Accelerated Design of Functional Materials:

Overcoming the “Valley of Death” in Heterogeneous Catalysis

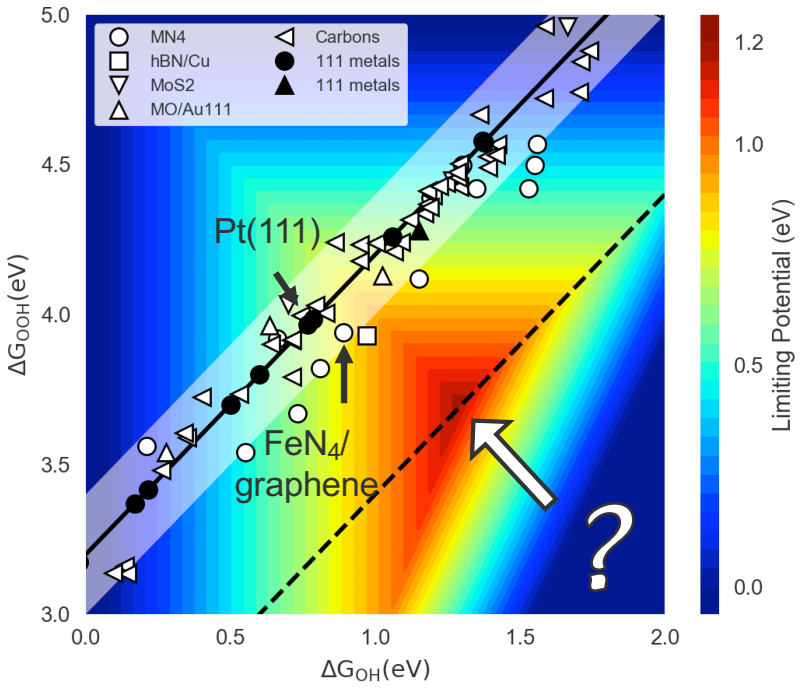
Prof. Ambar Kulkarni
University of California Davis

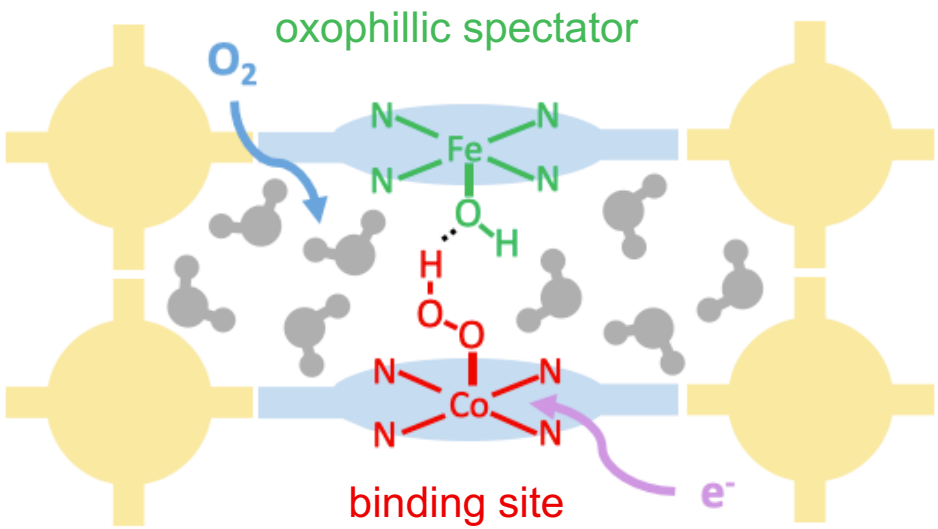
DS/ML Forum | Mar 4, 2025

Example 1: Theory-guided design of better of fuel cell catalysts

Ty Sours

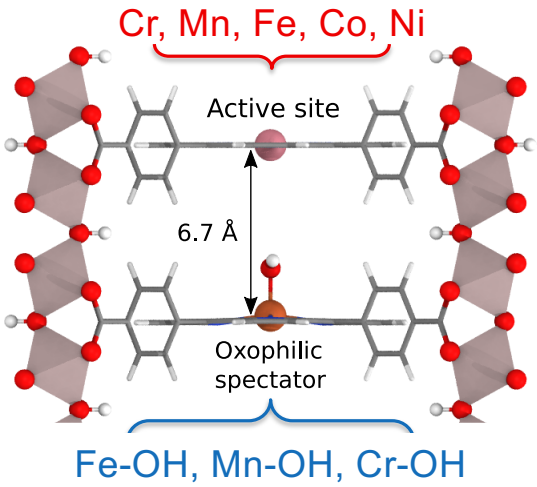
ORR performance is limited by the scaling relationships between *OOH and *OH

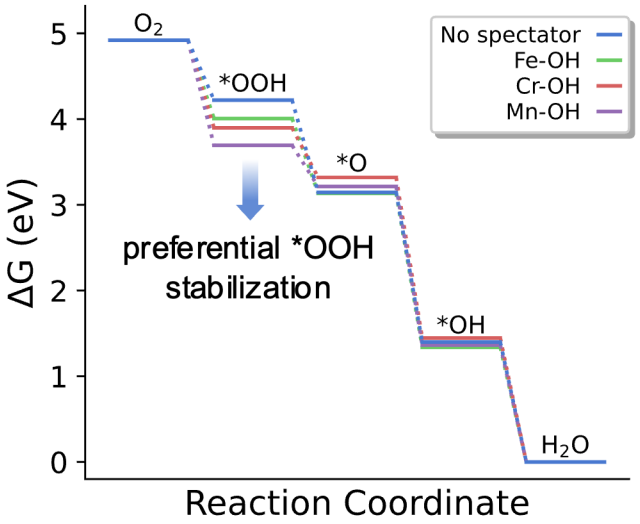


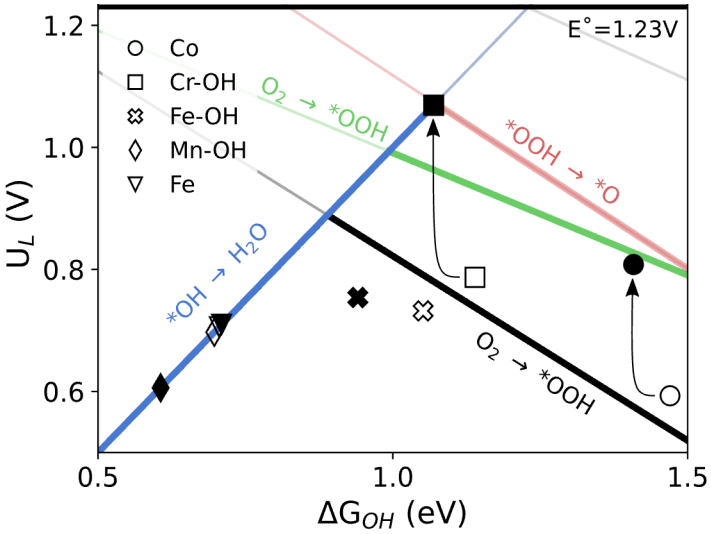


Kulkarni et al., *Chemical Reviews* **2018**

We identified several promising bimetallic PMOF materials …



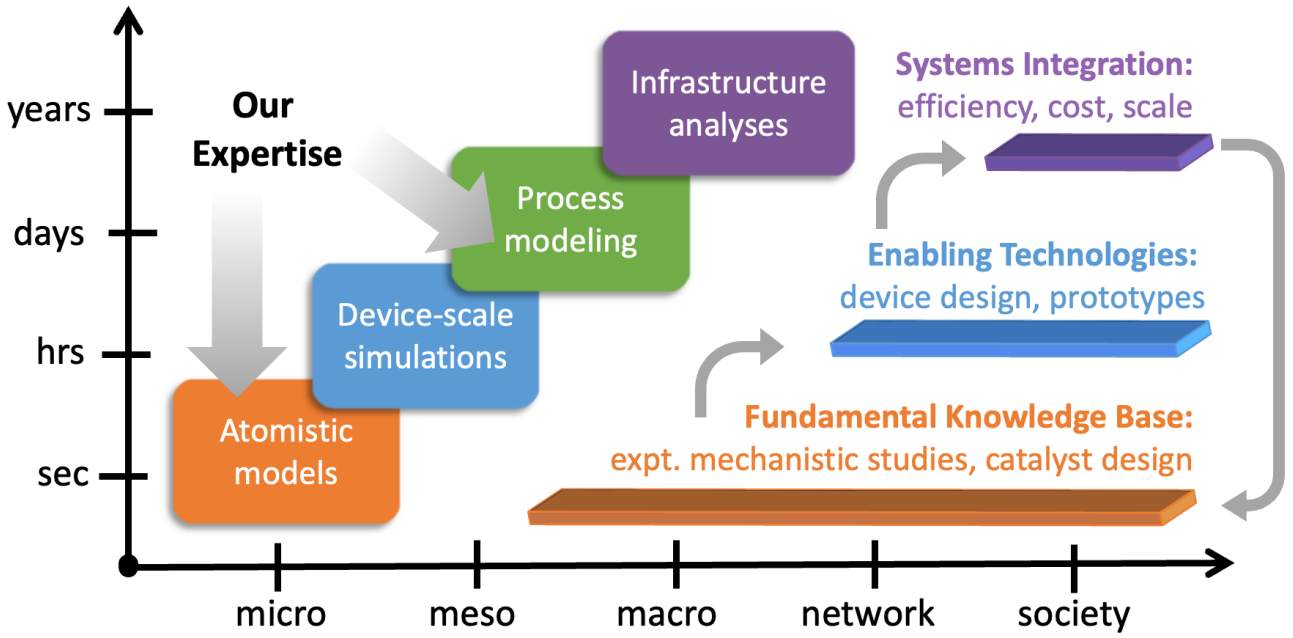




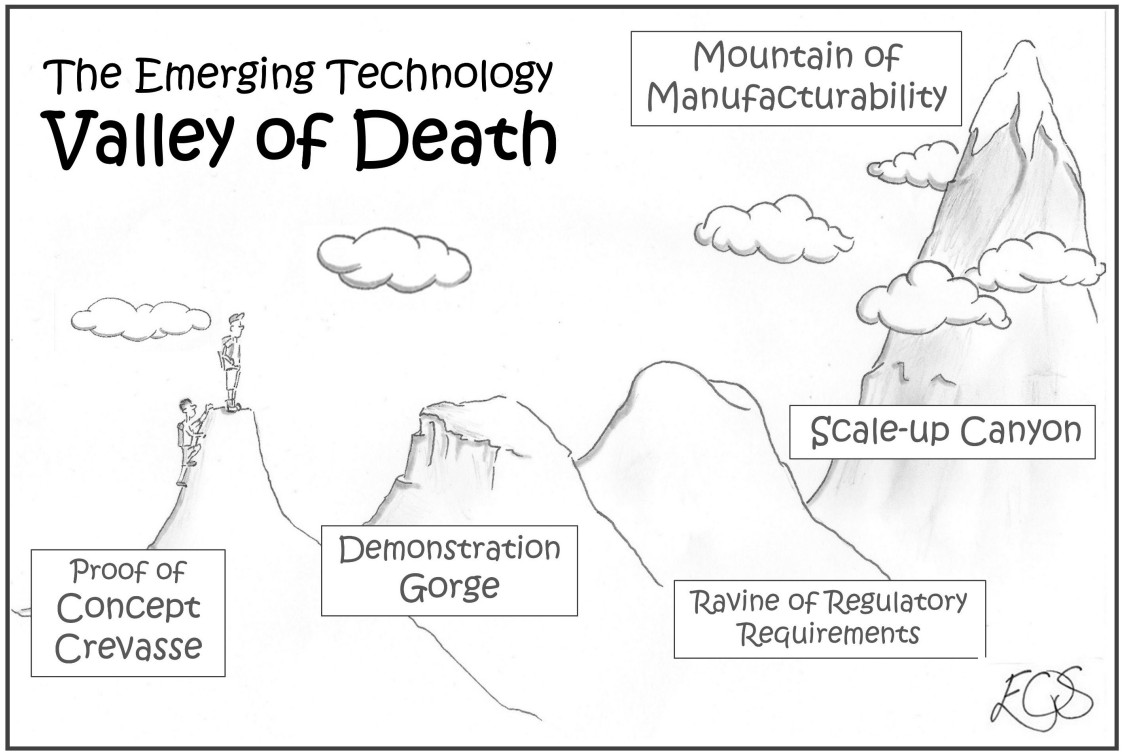
… but their synthesis was unsuccessful ☹

Sours et al., *JPCL* **2021**

Accelerate the development of new functional materials and novel processes using team-based academic, national lab, and industrial collabs.

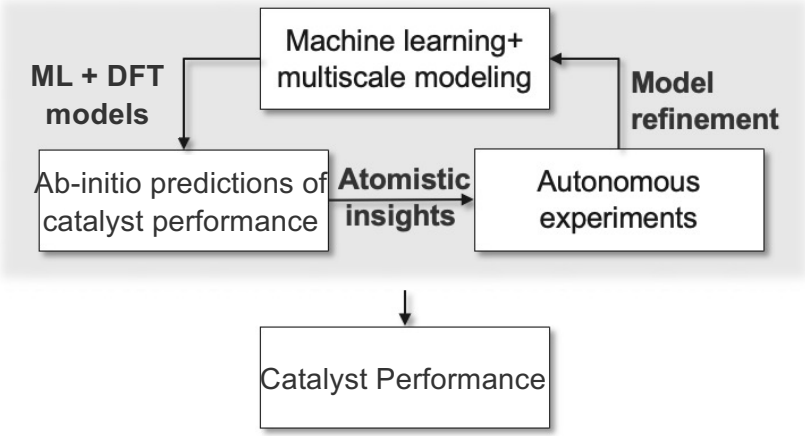


Overcoming the "Valley of Death" in Heterogenous Catalysis



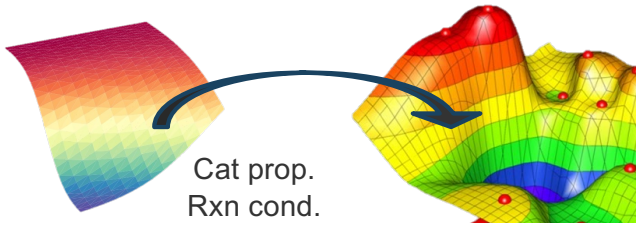
(a) The "big data" approach

(b) A physics-informed but data-driven strategy

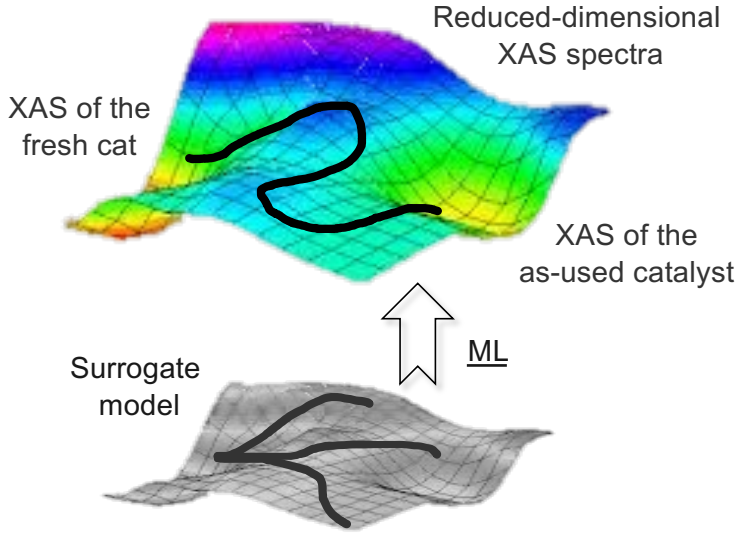


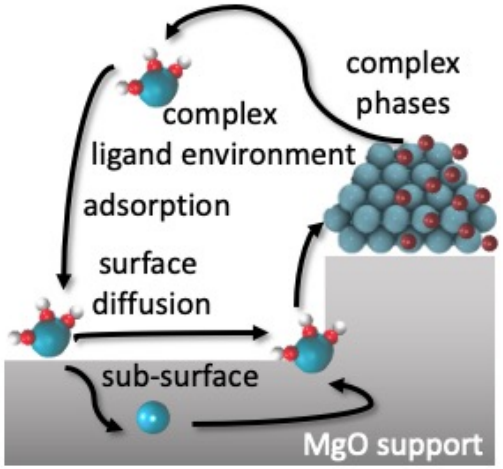
Applications to Catalyst Synthesis, Formed Materials, and Deactivation

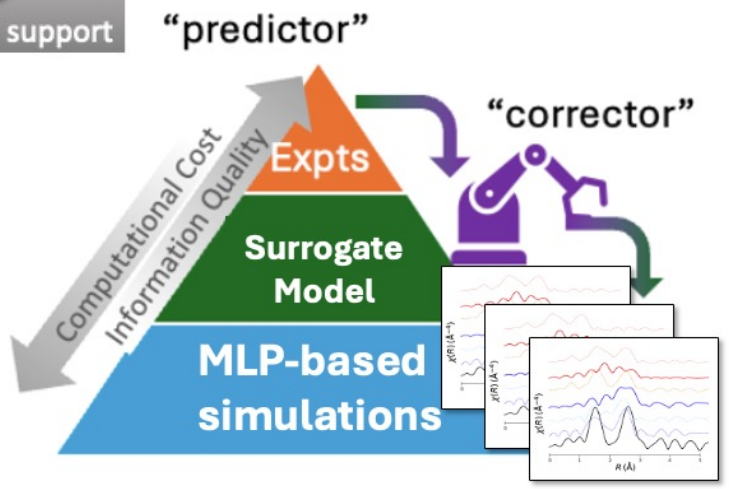
(a) Data-centric approach



(b) Structure-led approach

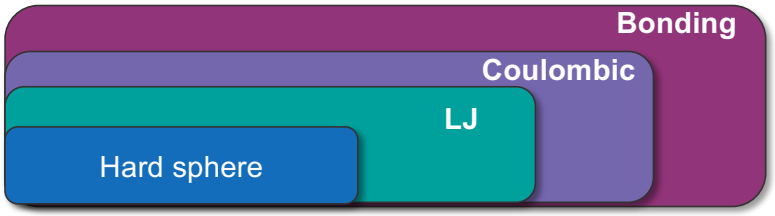


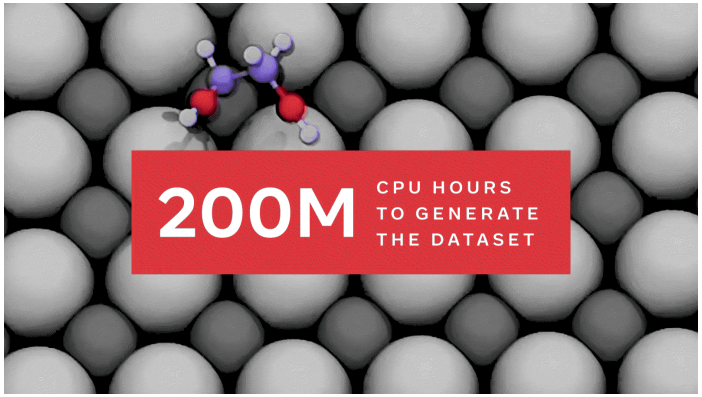


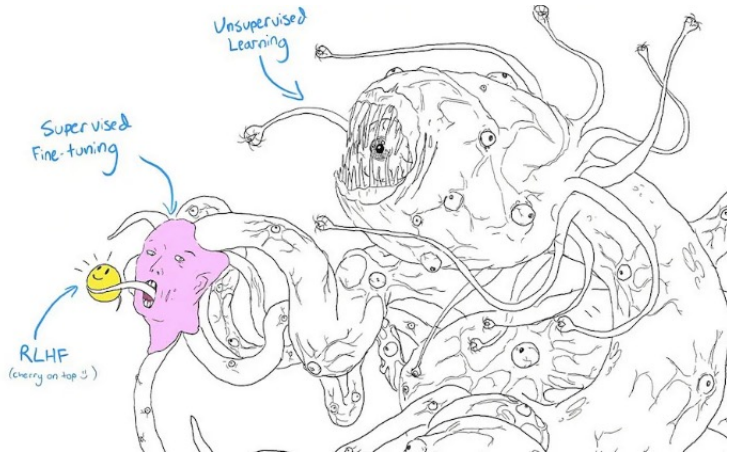


Open Problem 1: Foundational models for inter-atomic interactions that can be interpreted visually

- Machine learning potentials are now being trained on massive quantum chemistry datasets to develop "foundational" models.
- I would like to develop interpretable foundational models using curriculum learning that "teaches" an *as-simple-as-possible model* concepts of increasing complexity







Open Problem 2: How does information mold attention, and how can we rescue it?

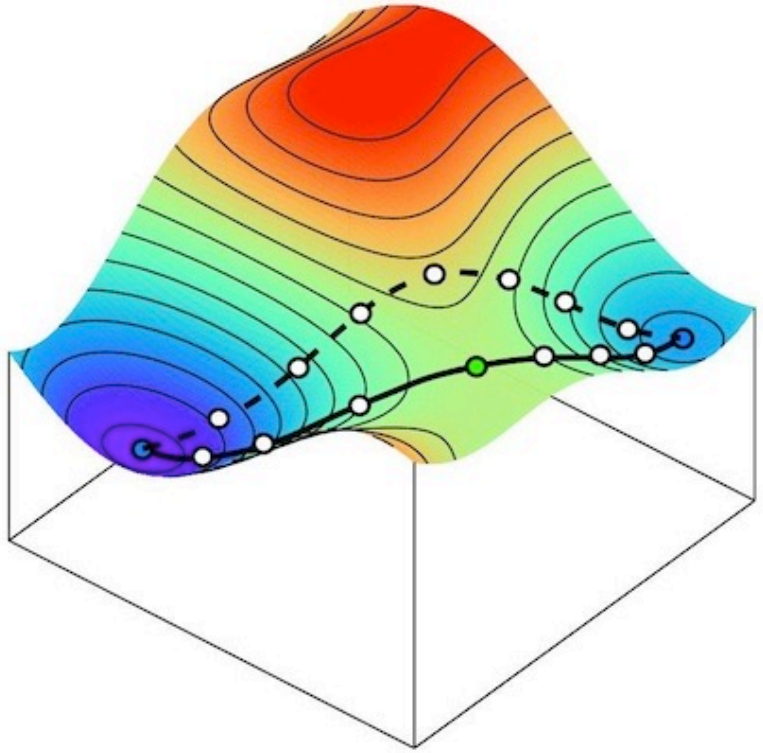
- Transition state theory can be used to obtain rates of individual elementary steps to predict macroscopic observables
- Systems (molecs, etc.) are driven to
  - decrease enthalpy

  (more stable, less unhappy)
  - maximize entropy

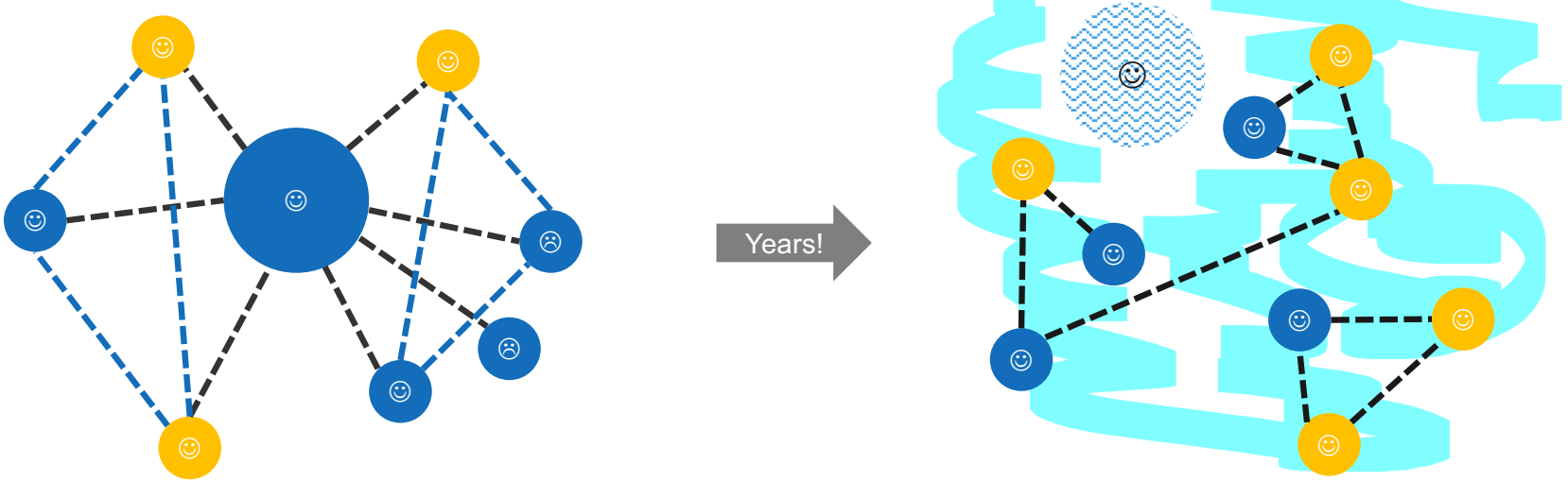
  (more freedom, flexibility)

- None of this matters ..

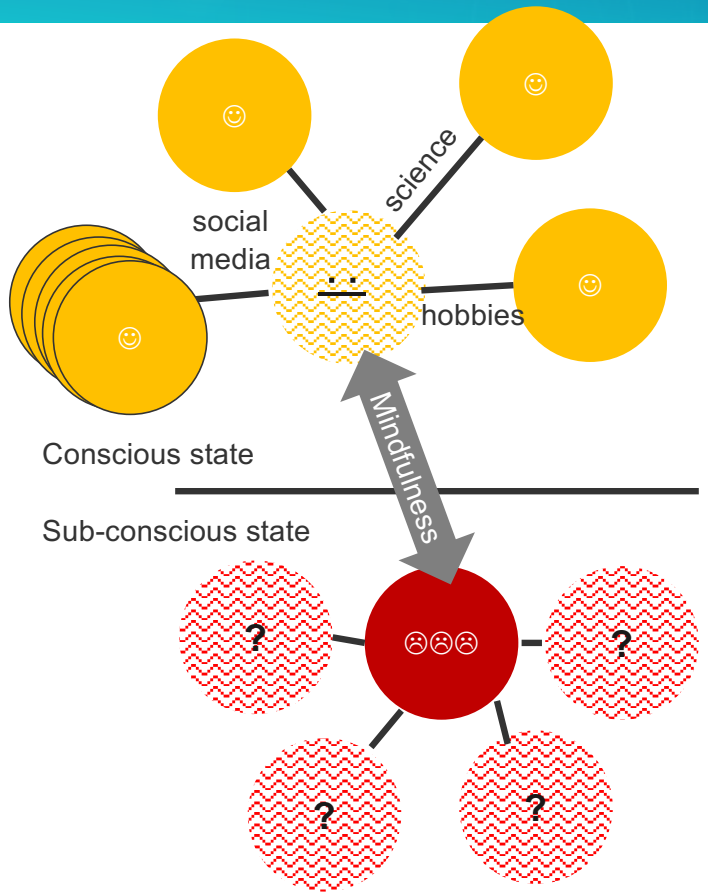
  .. unless We change how We live our lives

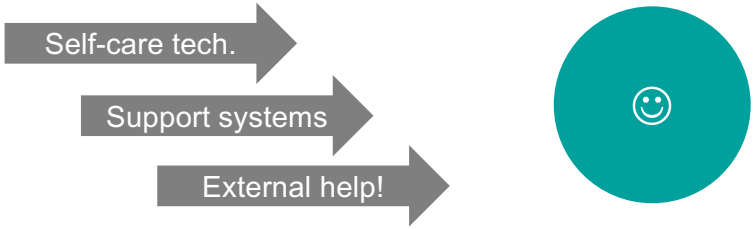


Nurture relationships ..



.. and take care of yourselves!





We need physics-based, easy to understand, foundational models that describe our inter-subjective perspectives *(and save our institutions from AI)*