

# Digitalization Interdisciplinarity

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# „Digitalization“

- **Digitization:** Transitioning from analog to digital
- **Digitalization:** Making digitized information work for you
- **Digital transformation:** Taking advantage of digitalization to create completely new (business) concepts

# Disciplinarity origins from „thought-styles“

- A thought collective, a term originated in German as "Denkkollektiv" by Ludwik Fleck, is a community of researchers who interact collectively towards the production or elaboration of knowledge using a shared framework of cultural customs and knowledge acquisition.

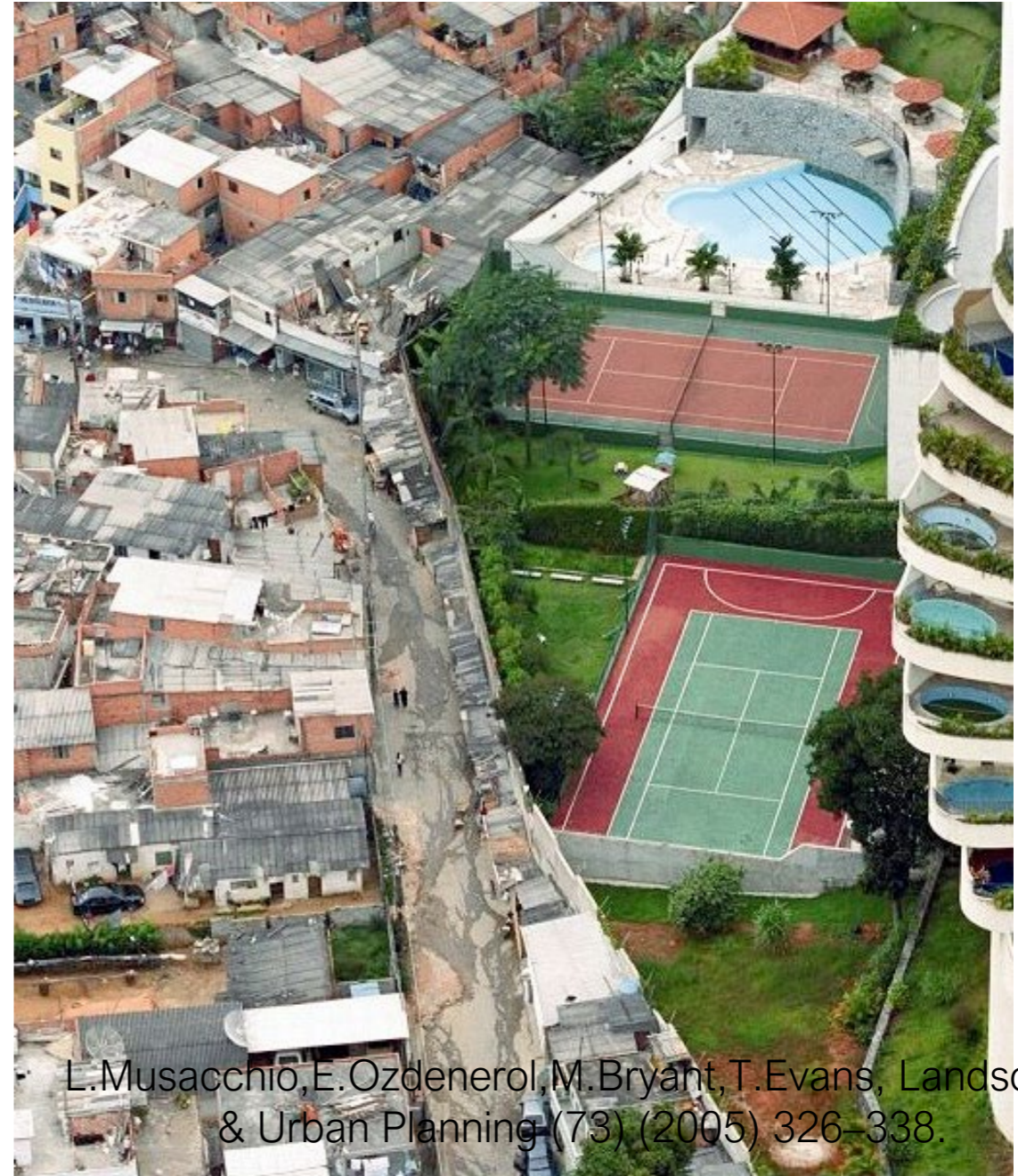
- Fleck, Ludwik. Entstehung Und Entwicklung Einer Wissenschaftlichen Tatsache: Einführung in Die Lehre Vom Denkstil Und Denkkollektiv. Basel: B. Schwabe, 1935



# history of ideas

- “the real problems (of society) do not come in discipline-shaped blocks”

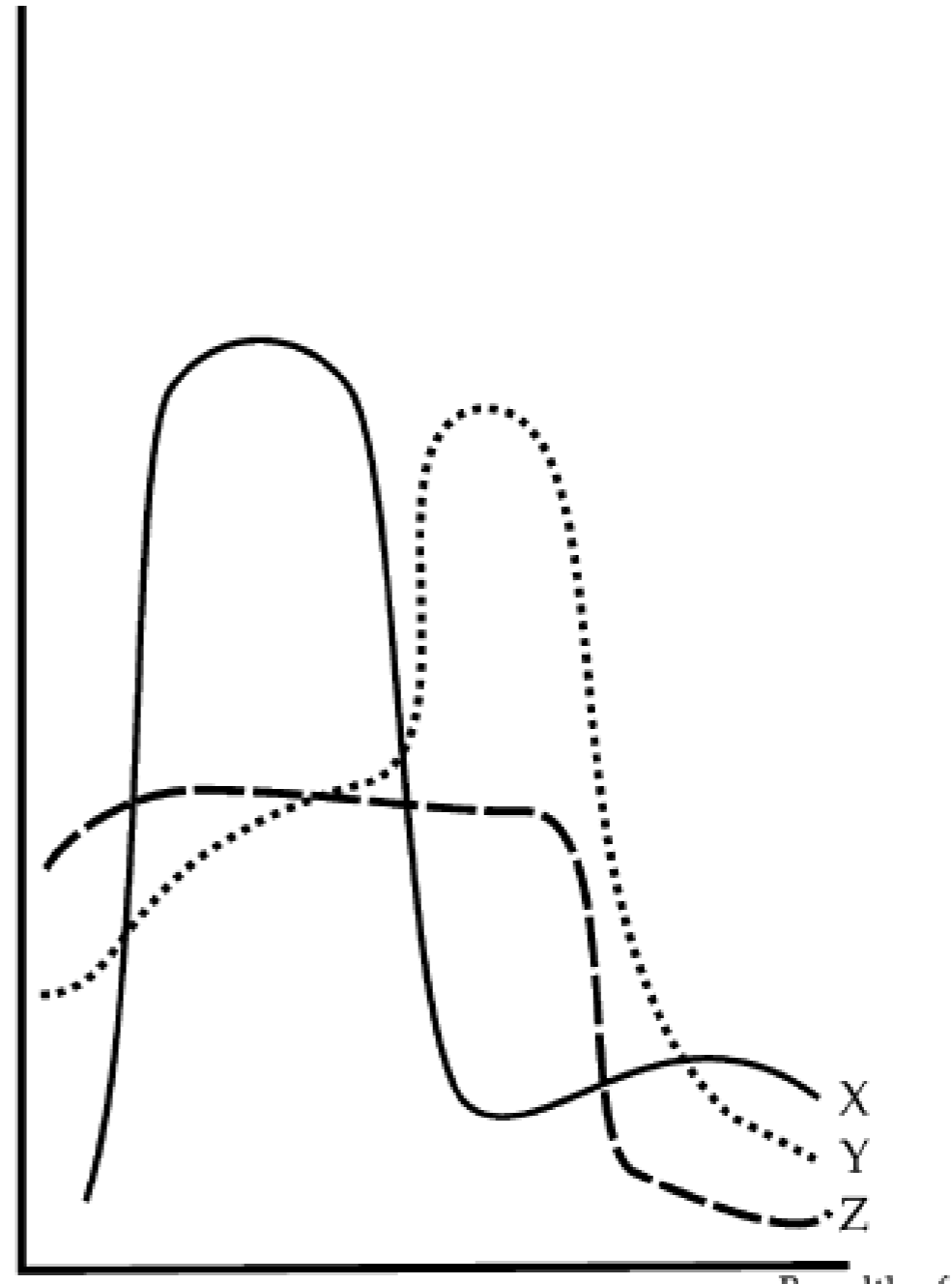
***new disciplines may emerge...  
..and they have!***



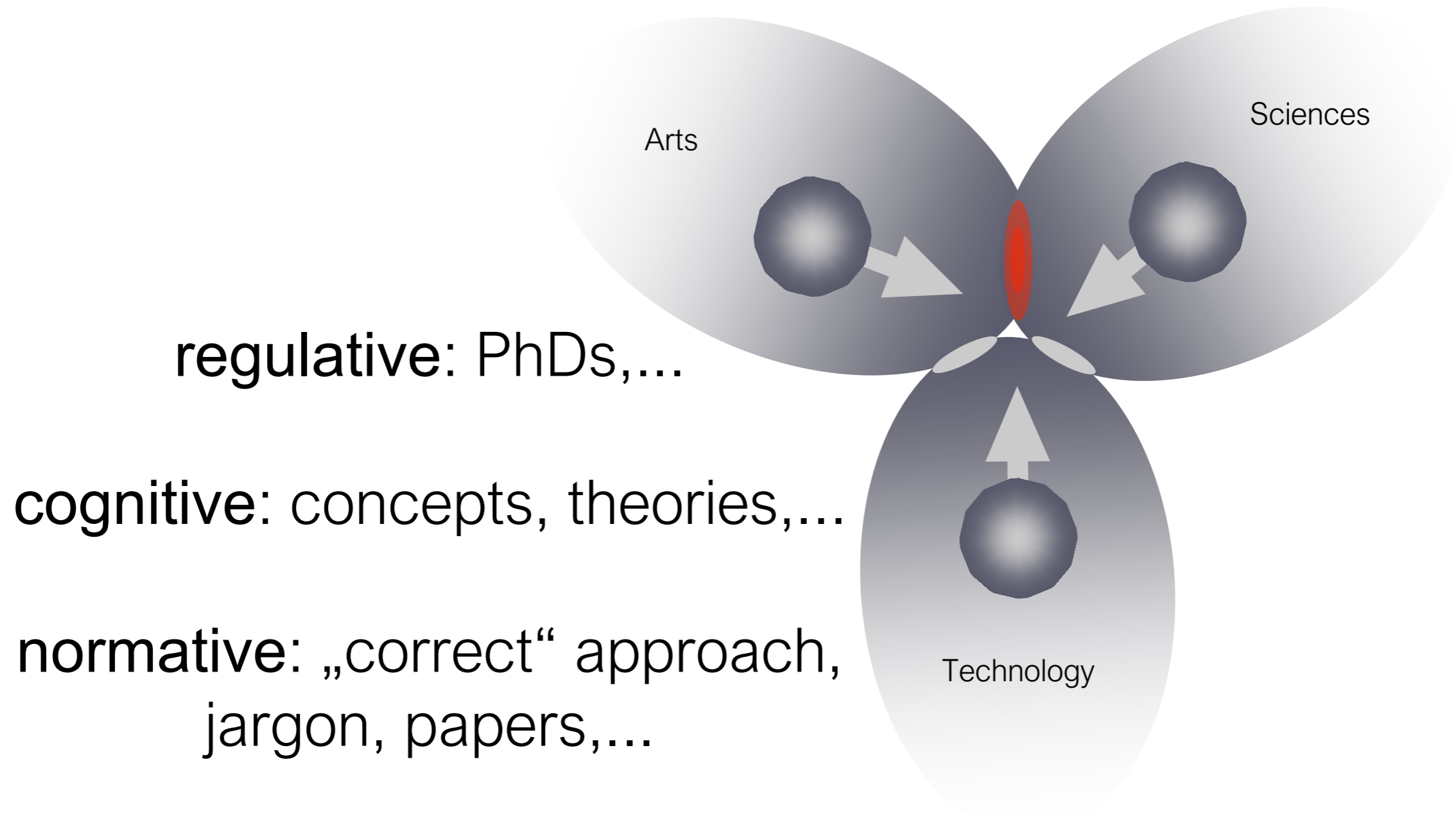
L.Musacchio, E.Ozdenerol, M.Bryant, T.Evans, Landscape & Urban Planning (73) (2005) 326–338.

# interdisciplinarity comes in various forms

- ID is not necessarily superficial
- one can be more or less narrow within a single discipline.
- Few individuals would know all of what a discipline contains.
- depends on how much time and effort one is willing to and able to spend on the other discipline

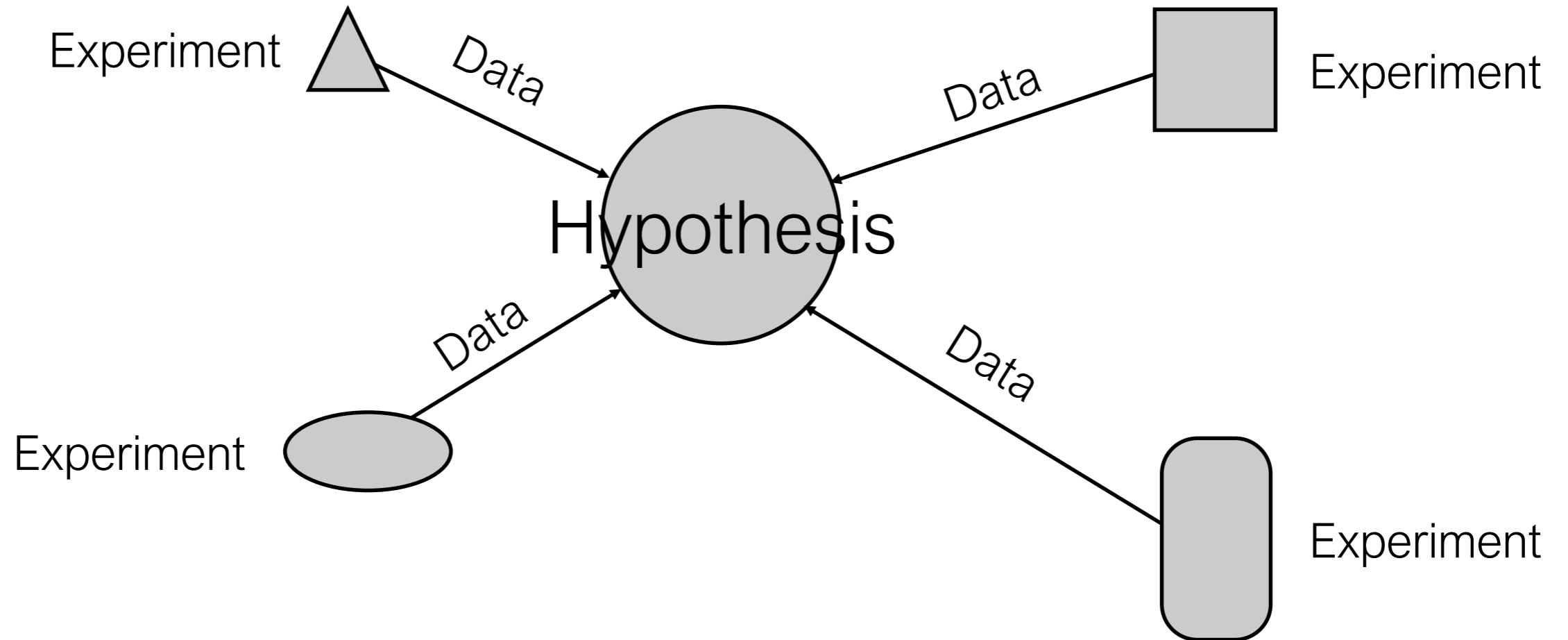


# Barriers against interdisciplinarity



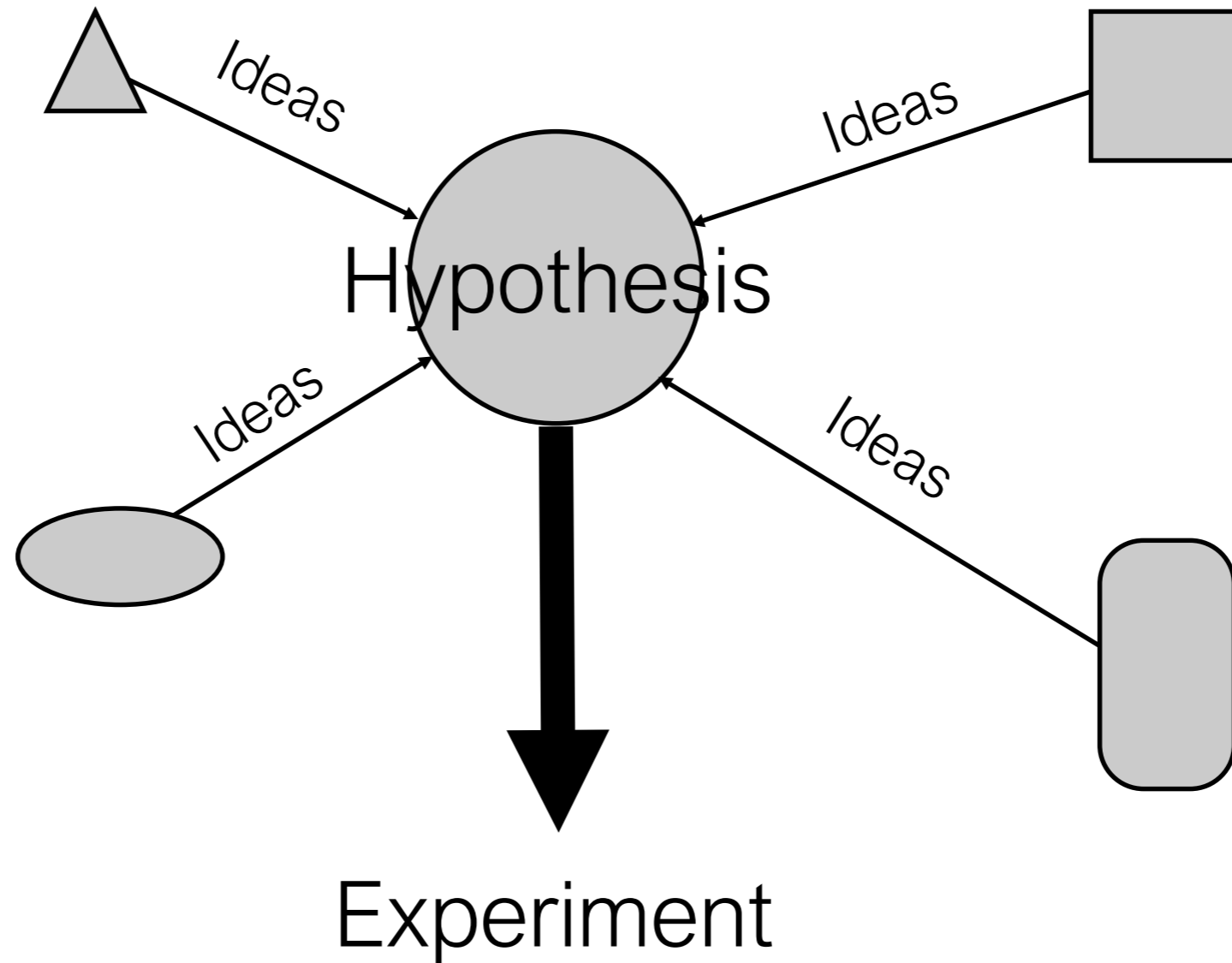
top-down: „indirect“ interdisciplinarity

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bottom-up: „direct“ interdisciplinarity

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## challenging a paradigm in sociology of science

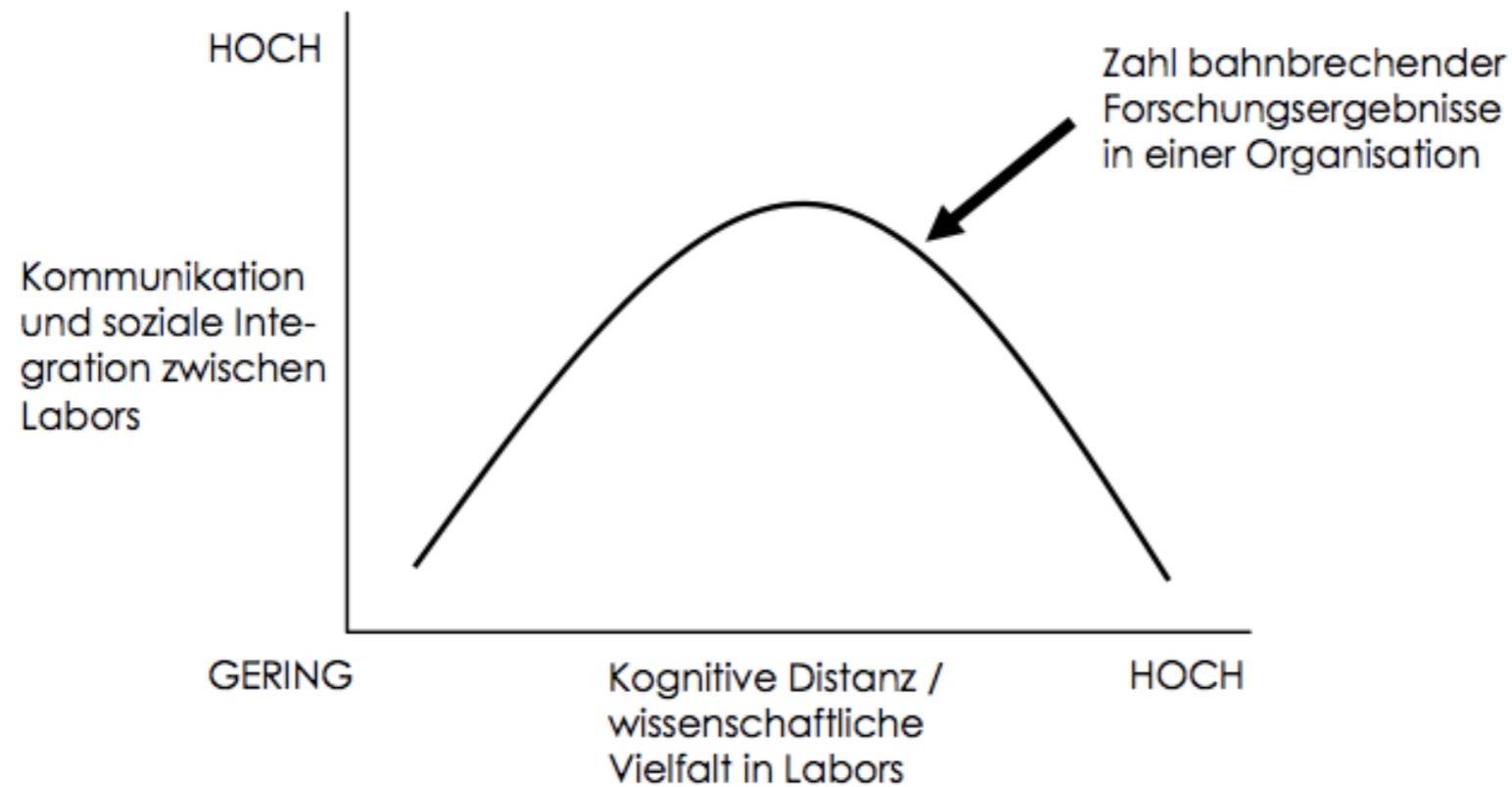


Abbildung 3. Moderate Disziplinenvielfalt in Kombination mit hoher sozialer Integration steht in positivem Zusammenhang mit der Anzahl der bahnbrechenden Forschungsergebnisse in biomedizinischen Forschungseinrichtungen (nach Hollingsworth, 2007, p. 133).

# Interdisciplinarity for one Brain

- ID does not need two individuals or more...
- ...it needs curiosity and translation.
- („digitalized“) translation provides a collective (scientific) experience
- ...unrestricts individual imagination
- ...may become a fundamental change of sociology of science

# Translation

digitized collective experience of a discipline ( publications, graphs, notions, equations, algorithms....)

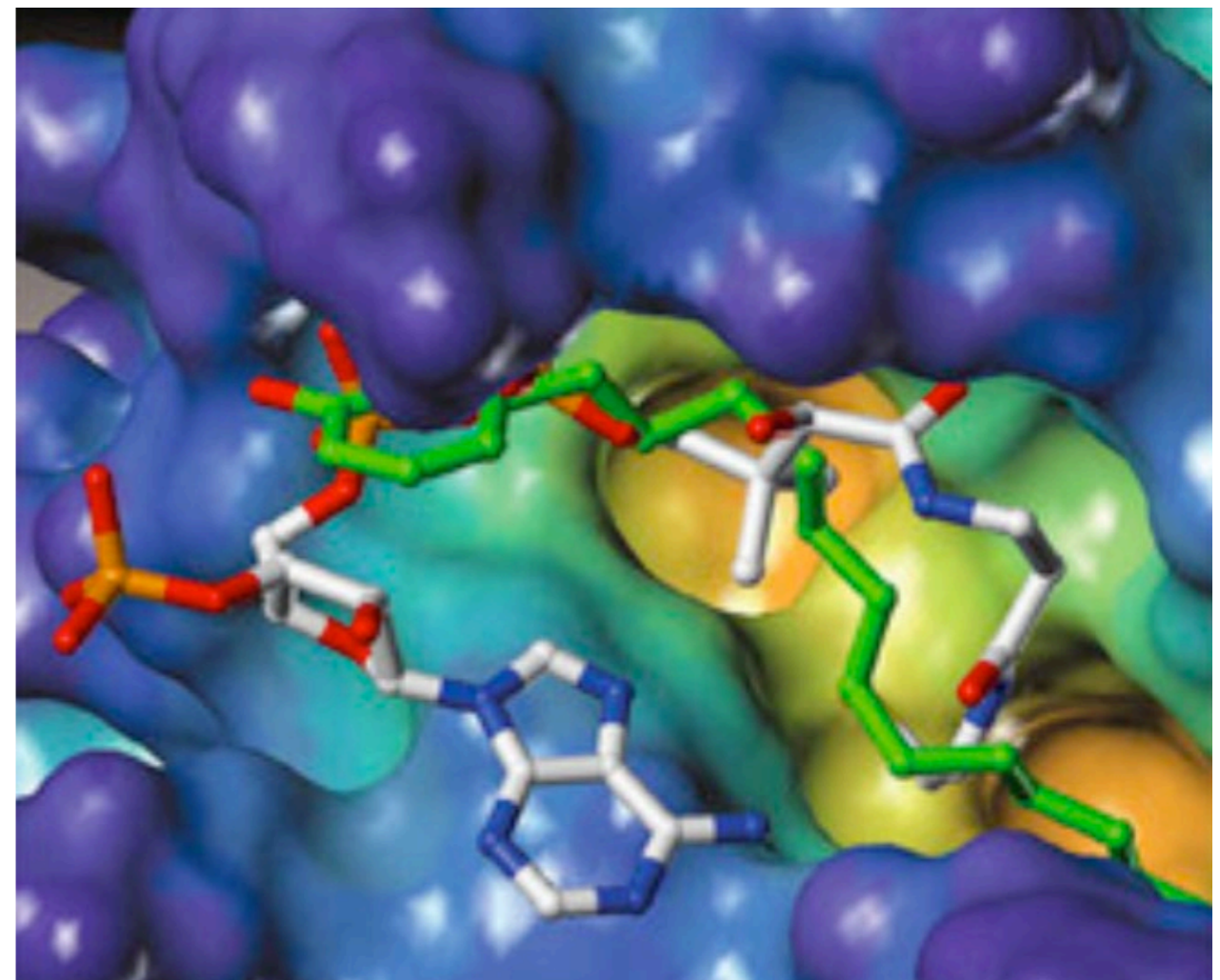
digitalized

**Digital Transformation**

sampling/mapping space  
(simulations, real experiments),  
low cost, fast

# drug design

„...as a key fits into a lock...“



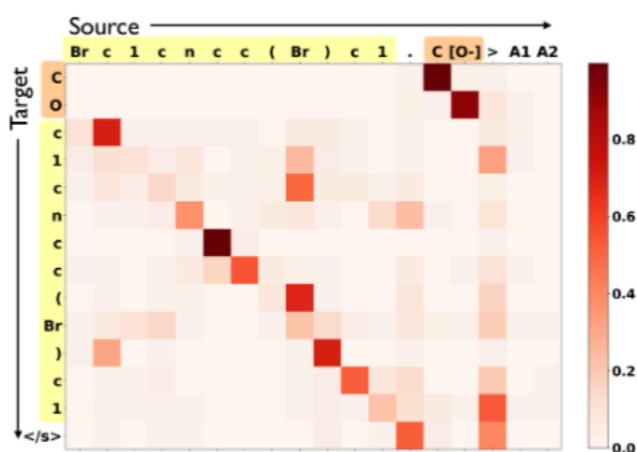
# “Found in Translation”: Predicting Outcomes of Complex Organic Chemistry Reactions using Neural Sequence-to-Sequence Models

Philippe Schwaller, Théophile Gaudin, Dávid Lányi,, Costas Bekas,, Teodoro Laino, IBM Research, Zurich

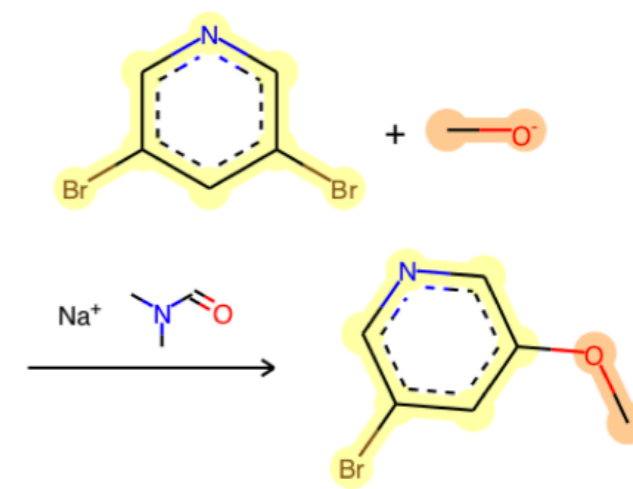
{phs,tga,dla,bek,teo}@zurich.ibm.com

„There is an intuitive analogy of an organic chemist’s understanding of a compound and a language speaker’s understanding of a word. Consequently, it is possible to introduce the basic concepts and analyze potential impacts of linguistic analysis to the world of organic chemistry.“

Attention is the key to take into account complex long-range dependencies between multiple tokens. Specific functional groups, solvents or catalysts have an impact on the outcome of a reaction, even if they are far from the reaction center in the molecular graph and therefore also in the SMILES string. Figure 2 shows how the network learned to focus first on the C[O<sup>-</sup>] molecule, to map the [O<sup>-</sup>] in the input correctly to the O in the target, and to ignore the Br, which is replaced in the target.



(a) Attention weights



(b) Reaction plotted with RDKit [27]

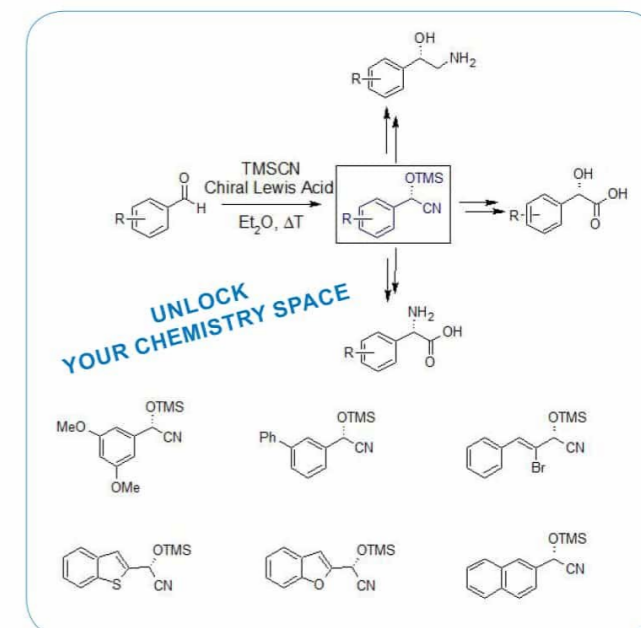
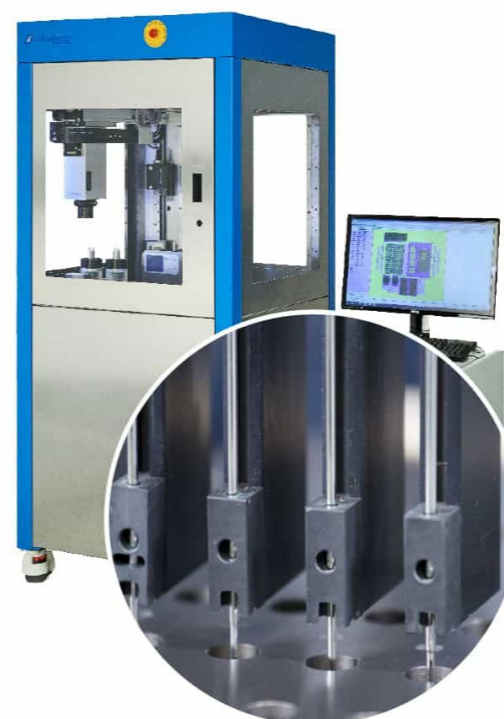
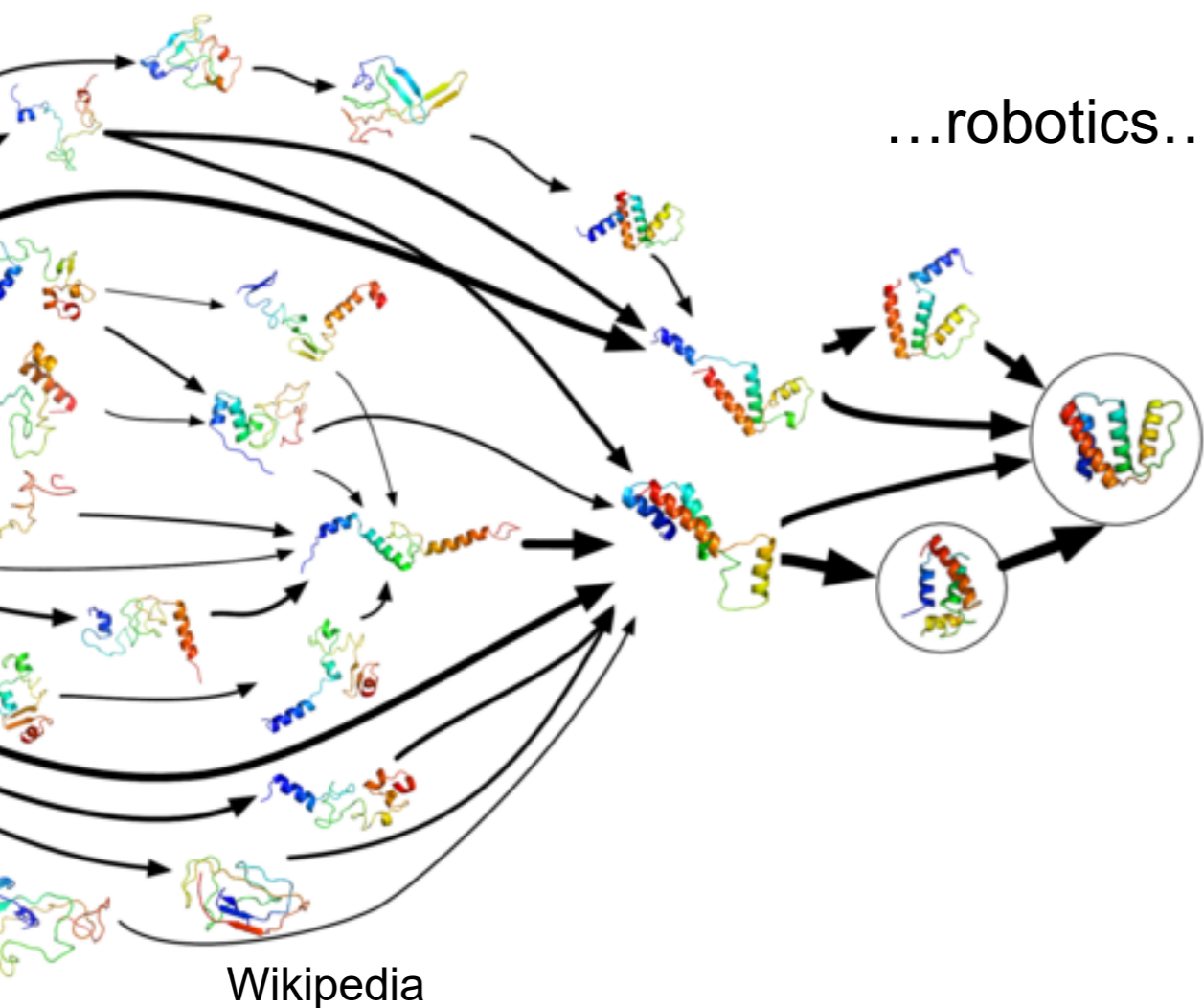
Figure 2: Reaction 120 from Jin’s USPTO test set. The atom mapping between reactants and product is highlighted. SMILES: Br c 1 c n c c ( Br ) c 1 . C [O-] > CN(C)C=O.[Na+] > COc1cncc(Br)c1

# Translation

digitized collective experience of a discipline (publications, graphs, notions, equations, algorithms....)

advanced computing,...

...robotics...

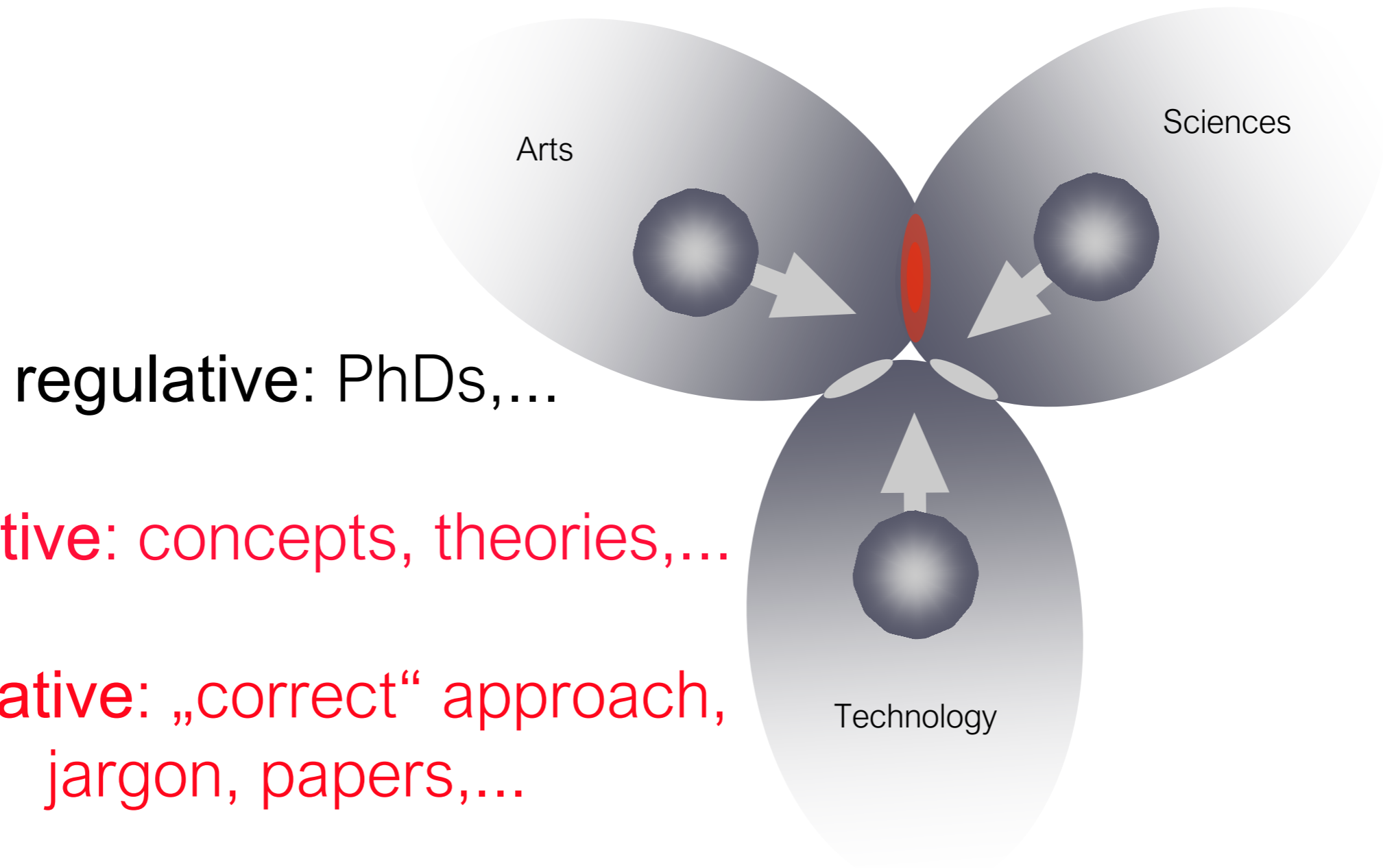


## Example Workflow:



sampling/mapping space  
(simulations, real experiments),  
low cost, fast

# Barriers against interdisciplinarity



**Digital Transformation**