Institute for Advanced Studies
in Basic Sciences
Gava Zang, Zanjan, Iran

Reactivity Scales Prediction Model for Ionic Liquids Using Machine Learning

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method

Outline!

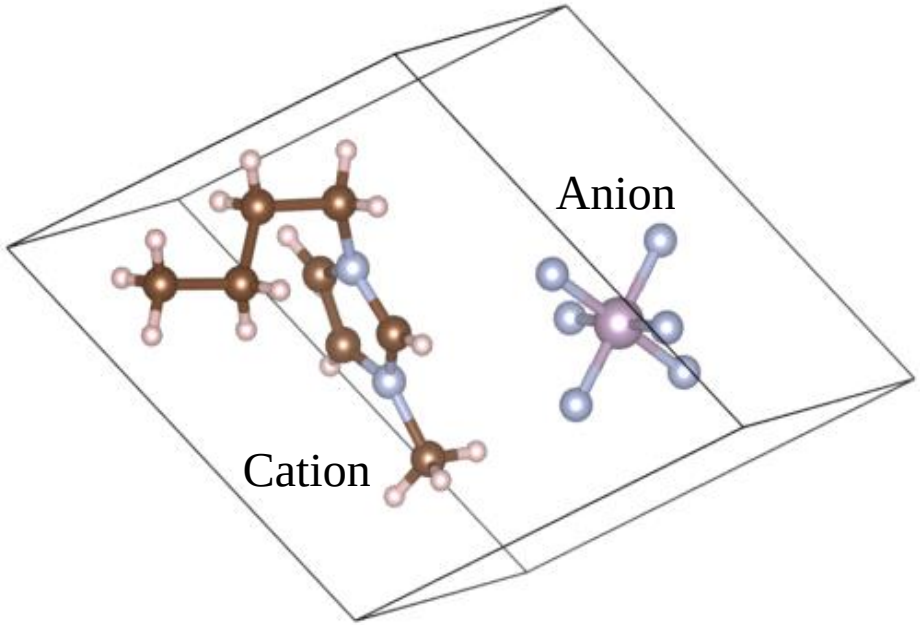
1

Room Temperature Ionic Liquids (RTILs)

2

Machine Learning (ML)

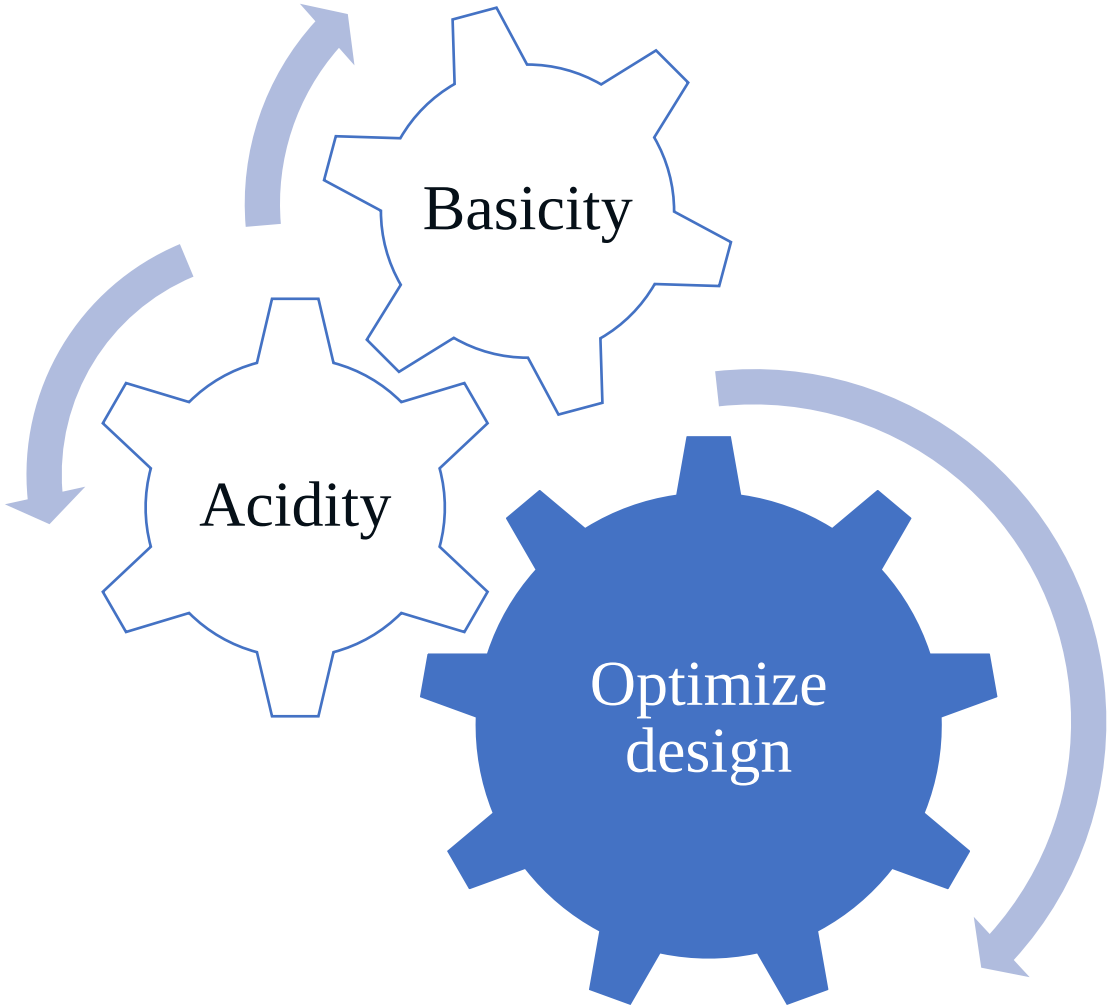
Room Temperature Ionic Liquids (RTILs)

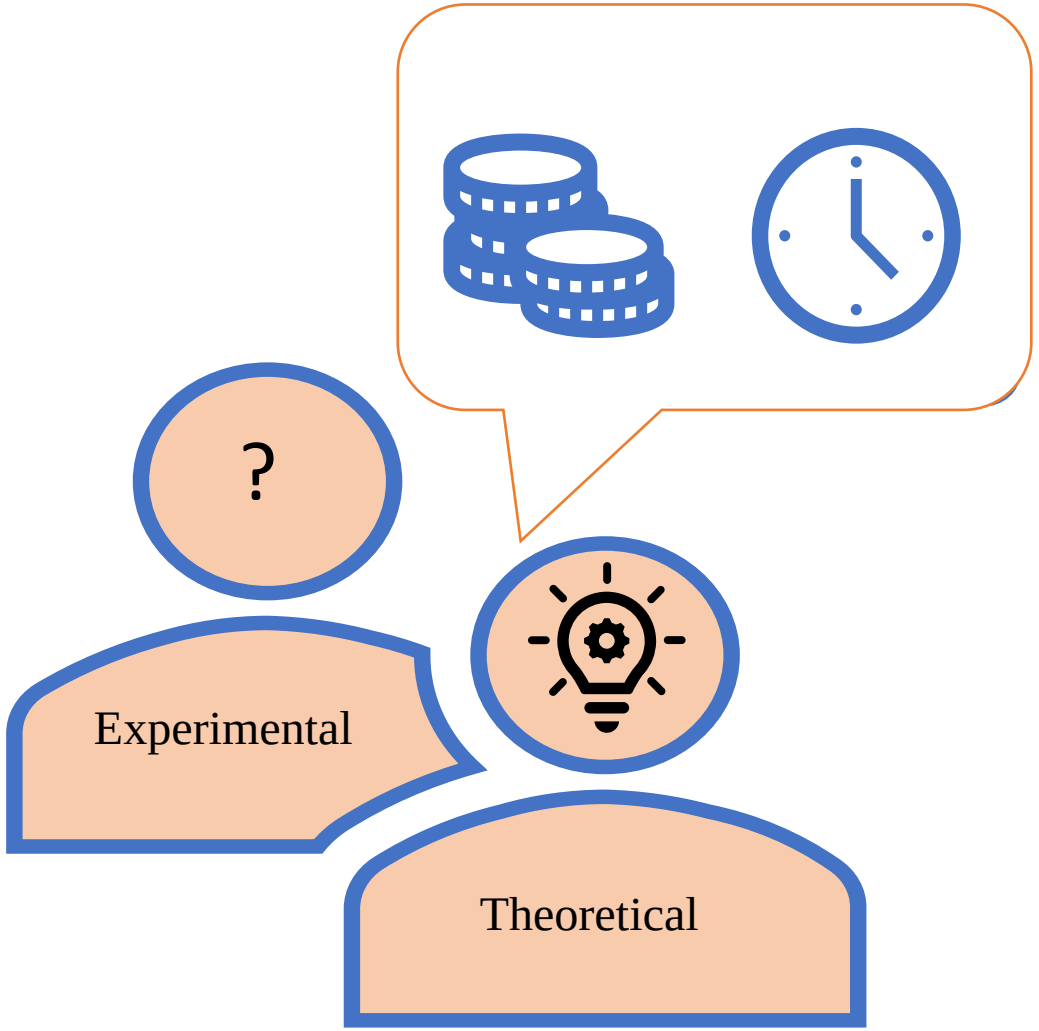


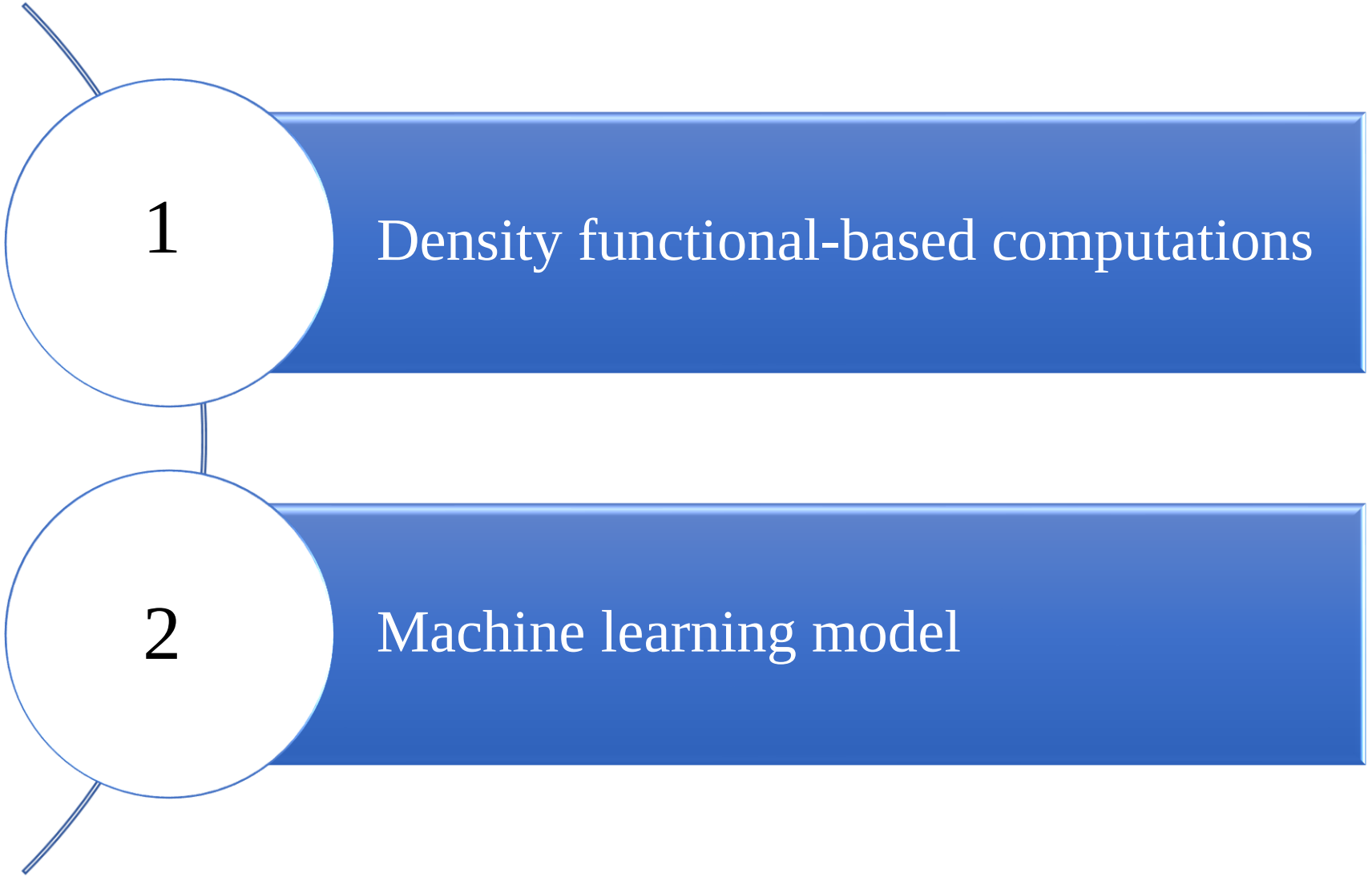
- Low corrosivity
- Less propensity for hydrolysis
- Being inflammable
- Less toxic
- Offering enhanced separation and recycling strategies

❖ **Being designable Combinations**

✓ (Solvents + Catalysis) application

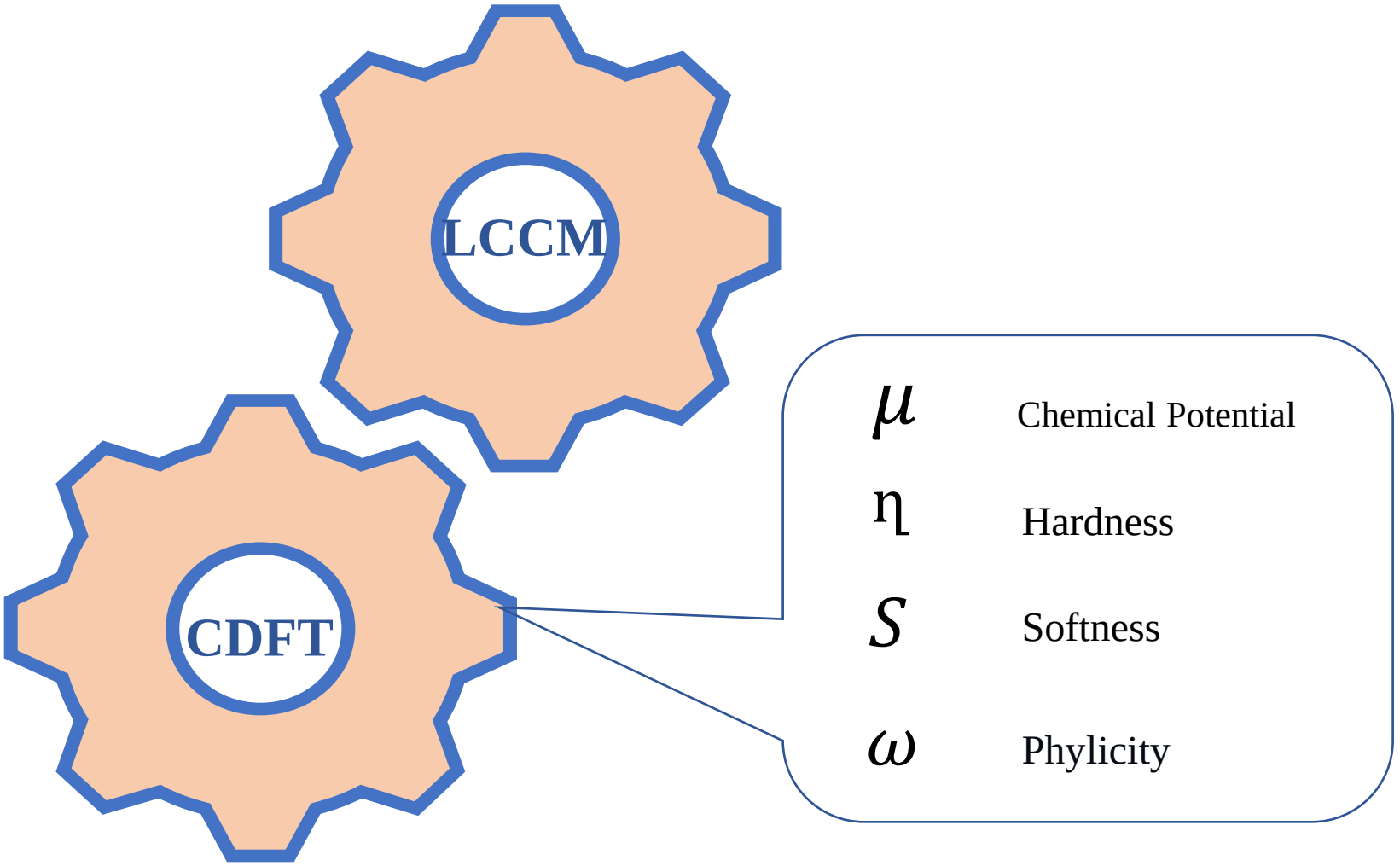

Basicity
Acidity
Optimize design


?
Experimental
Theoretical


1
Density functional-based computations
2
Machine learning model

Local Charge Capacity Model (LCCM)

- Focus on cation
- Plays role in understanding of the acid base properties
- Provides a framework for analysing and predicting the acid-base behaviour


LCCM
CDFT
μ Chemical Potential
η Hardness
S Softness
ω Phylicity

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

- Hartree-Fock (HF)
- Post-Hartree-Fock
- Density Functional Theory (DFT)

1- Downloading data from **PubChem**

2- Converting to the gaussian input

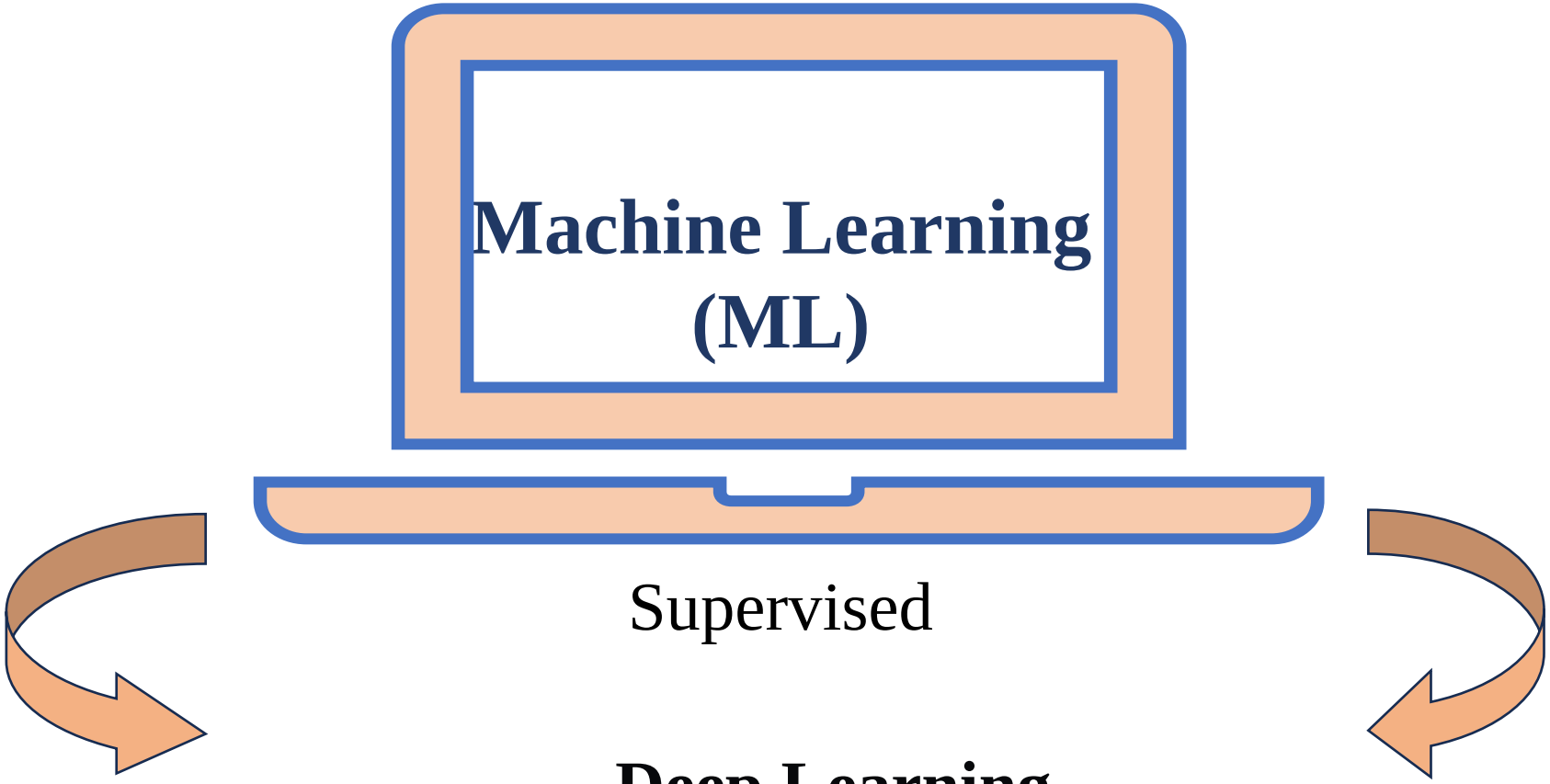
3- Optimizing data

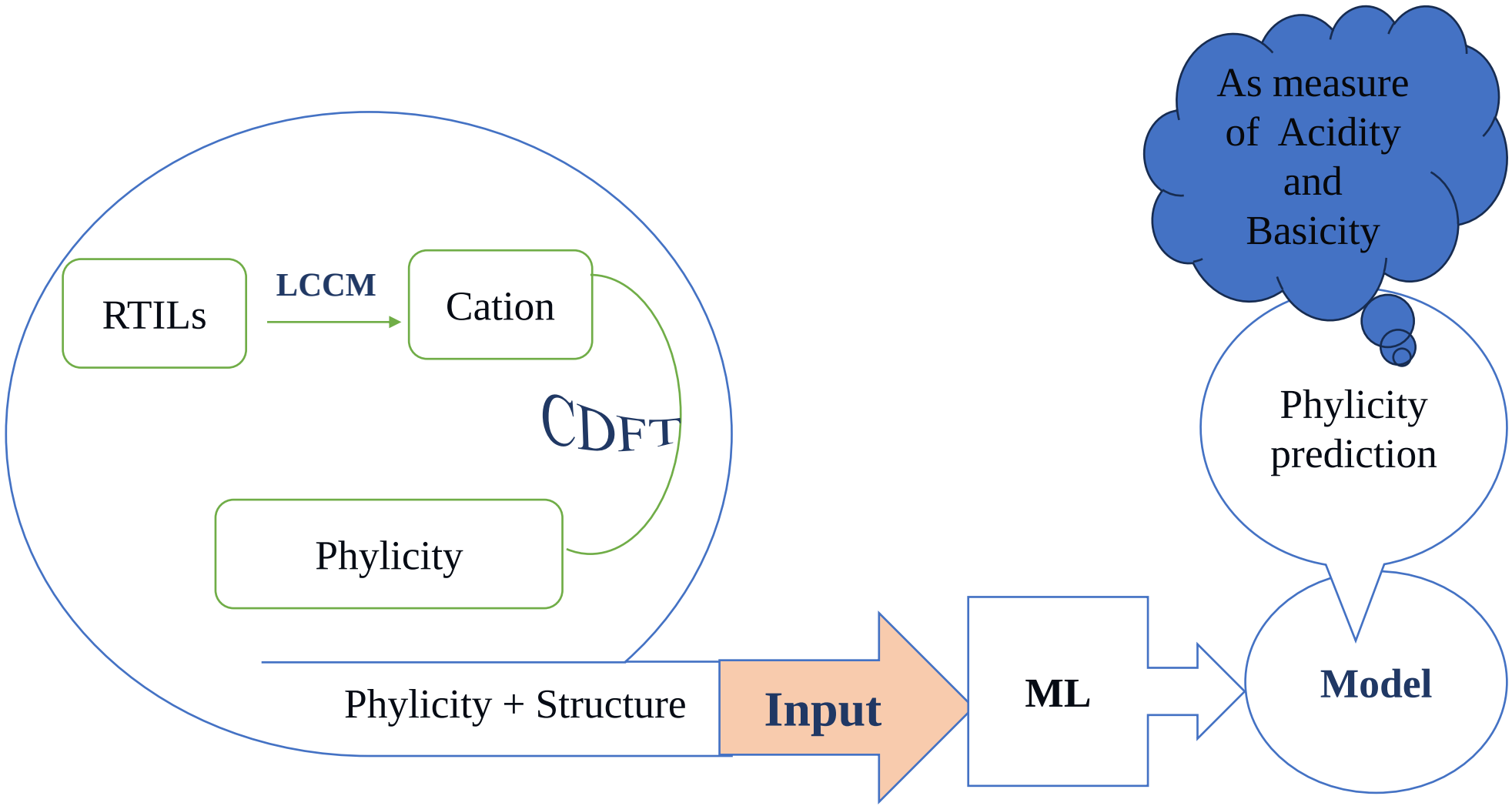
4- Extracting optimized data

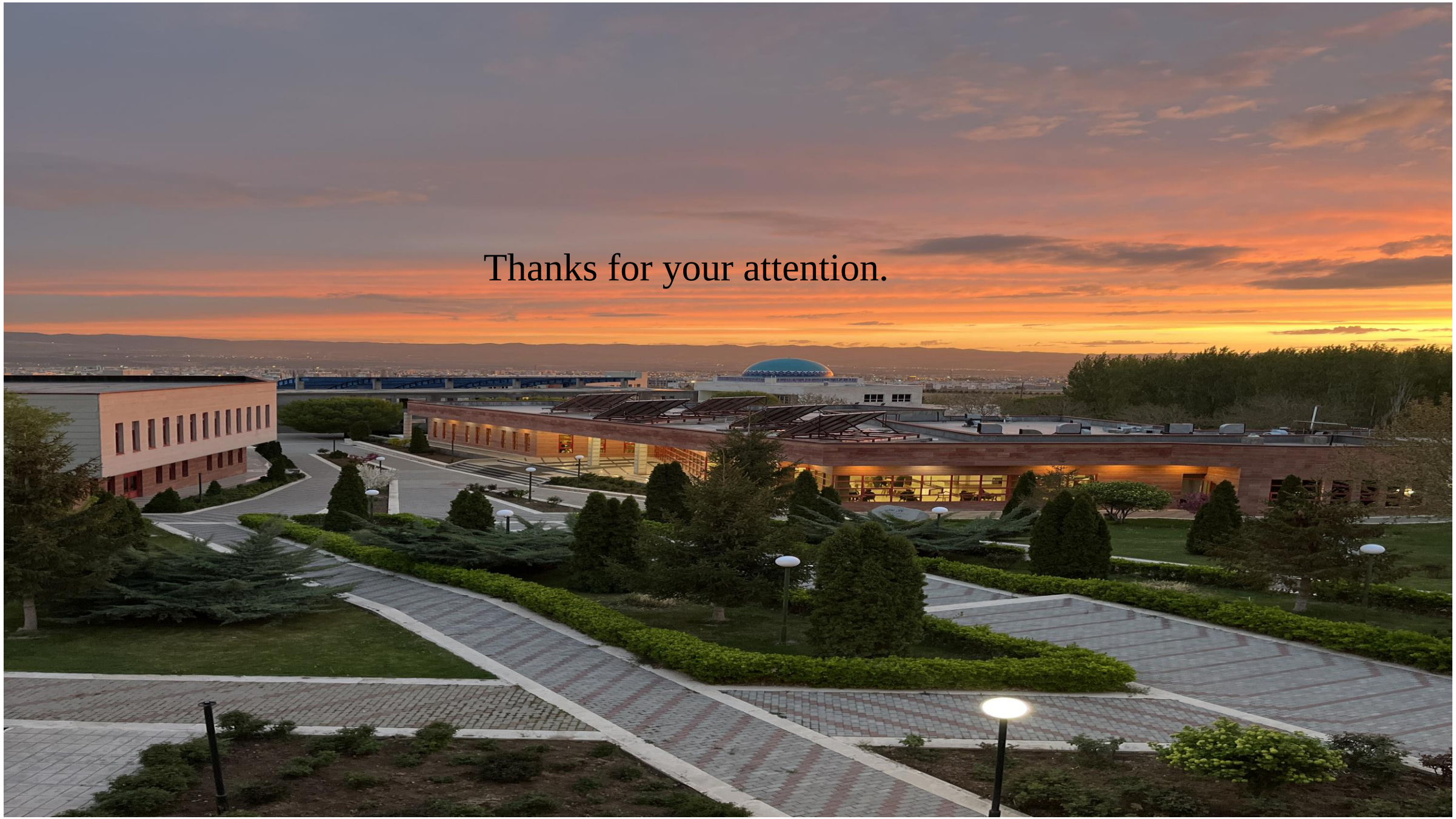
5- Computing CDFT data

6- Making final table

Compound	HOMO	LUMO	I	A	ω	μ	η	S	Δnmax
optimized_structure_2-C	-0.62413	-0.21496	0.62	0.21	-0.43	-0.42	-0.2	-4.89	-2.05
optimized_structure_8-C	-0.55214	-0.20216	0.55	0.2	-0.41	-0.38	-0.17	-5.71	-2.16
optimized_structure_10-C	-0.55321	-0.20047	0.55	0.2	-0.4	-0.38	-0.18	-5.67	-2.14
optimized_structure_1-C	-0.80099	-0.23402	0.8	0.23	-0.47	-0.52	-0.28	-3.53	-1.83
optimized_structure_18-C	-0.44265	-0.18216	0.44	0.18	-0.37	-0.31	-0.13	-7.68	-2.4
optimized_structure_9-C	-0.55167	-0.20365	0.55	0.2	-0.41	-0.38	-0.17	-5.75	-2.17
optimized_structure_6-C	-0.54346	-0.37783	0.54	0.38	-1.28	-0.46	-0.08	-12.08	-5.56


Machine Learning
(ML)
Supervised
Deep Learning


As measure of Acidity and Basicity
RTILs
LCCM
Cation
CDFT
Phylicity
Phylicity prediction
Phylicity + Structure
Input
ML
Model


Thanks for your attention.