UNIVERSITÉ DU LUXEMBOURG

AIDD kick-off meeting

ESR13: Quantum machine learning for reactivity (WP3)

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Theoretical Chemical Physics group

Headed by Prof. Dr. Alexandre Tkatchenko

- Machine learning in Chemical Physics
- Non-covalent interactions
- Imaginary time path-integrals

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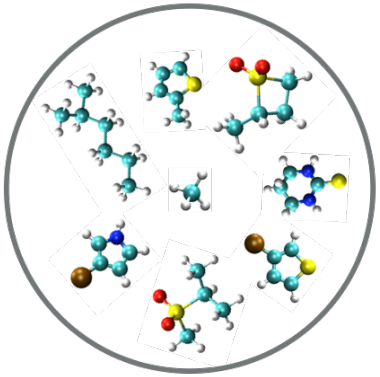
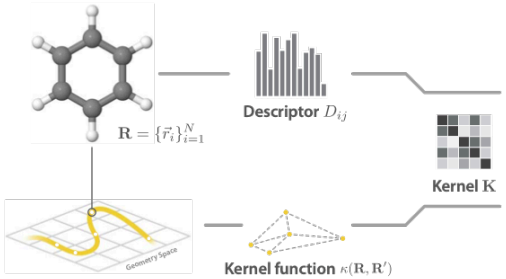
Molecular property prediction

QM7-X dataset

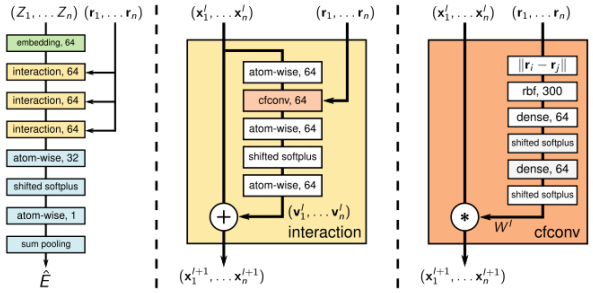


Physicochemical properties



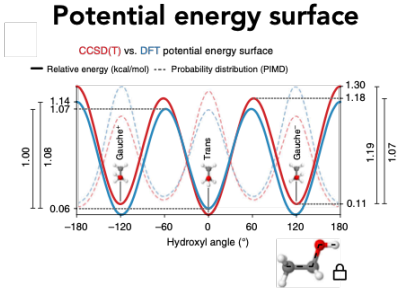
sGDML:
Kernel function

SchNet:
Neural Network

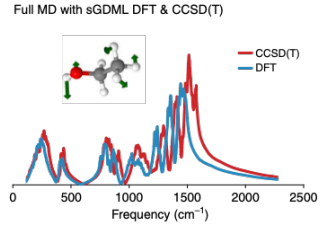


Machine learning model

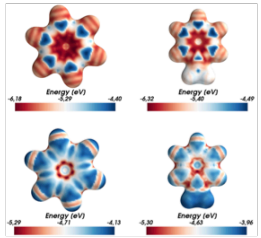
Potential energy surface



Vibrational spectra in nanoseconds



Local chemical potentials



K.T. Schütt, .., A. Tkatchenko, *Nat. Commun.*, 8, 13890, (2017).
S. Chmiela, .., A. Tkatchenko, *Nat. Commun.*, 9, 3887, (2018).
J. Hoja, .., A. Tkatchenko, *Scientific Data*, accepted, (2021).

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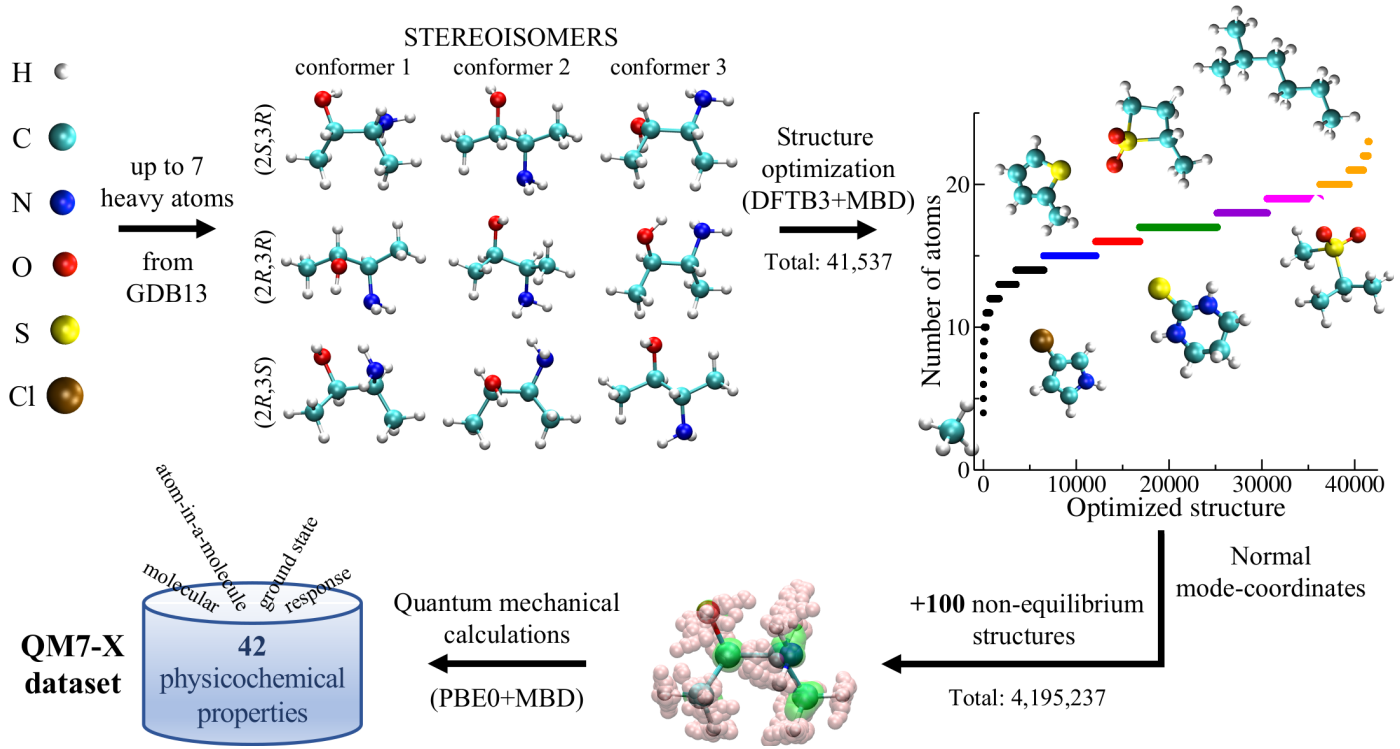
Dataset generation

- Small organic molecules up to 7 heavy atoms (QM7-X dataset)



- Small and large molecules with pharmaceutical relevance (UniLu-Janssen dataset)

Ongoing project in collaboration with Janssen Pharmaceutical.

J. Hoja, .., A. Tkatchenko, *Scientific Data*, accepted, (2021).

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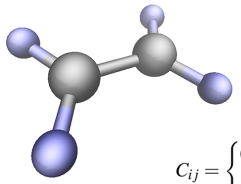
QM descriptors

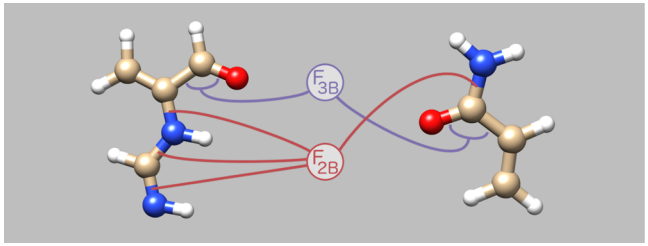
- Coulomb matrix



$$C_{ij} = \begin{cases} 0.5\, Z_i^{2.4} & \forall i = j \\ \frac{Z_i Z_j}{|\mathbf{R}_i - \mathbf{R}_j|} & \forall i \neq j. \end{cases}$$

$$\mathbf{C} = \begin{array}{c|cccccc} & \mathrm{H} & \mathrm{H} & \mathrm{C} & \mathrm{C} & \mathrm{H} & \mathrm{H} \\ \hline \mathrm{H} & 0.5 & 0.3 & 2.9 & 1.5 & 0.2 & 0.2 \\ \mathrm{H} & 0.3 & 0.5 & 2.9 & 1.5 & 0.2 & 0.2 \\ \mathrm{C} & 2.9 & 2.9 & 36.9 & 14.3 & 1.5 & 1.5 \\ \mathrm{C} & 1.5 & 1.5 & 14.3 & 36.9 & 2.9 & 2.9 \\ \mathrm{H} & 0.2 & 0.2 & 1.5 & 2.9 & 0.5 & 0.3 \\ \mathrm{H} & 0.2 & 0.2 & 1.5 & 2.9 & 0.3 & 0.5 \end{array}$$

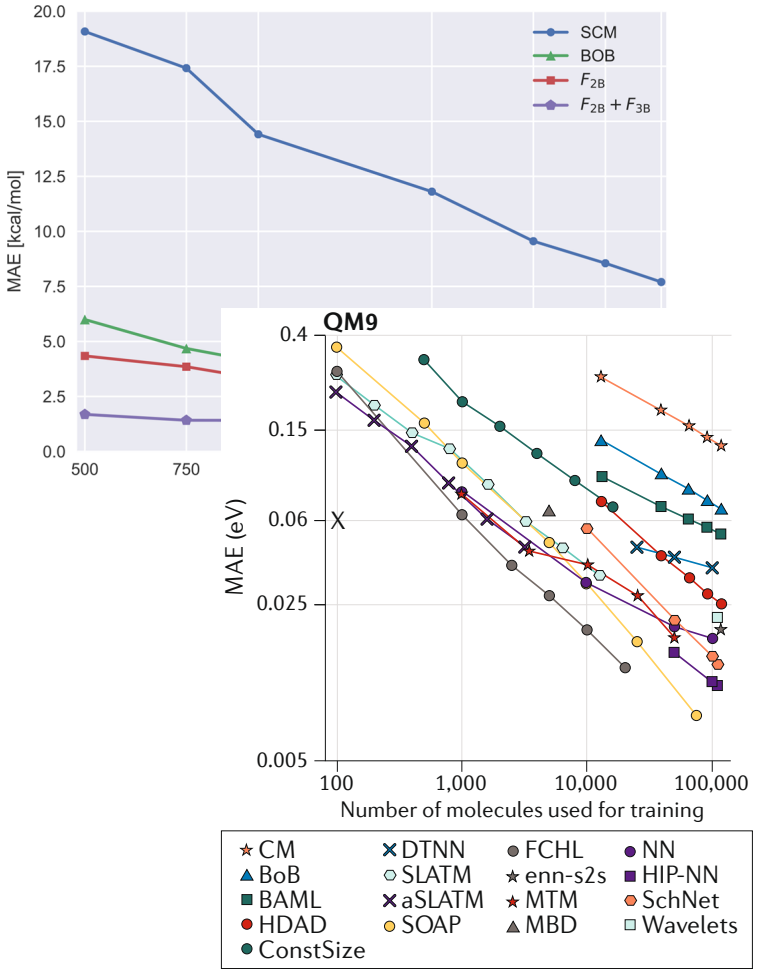
- Two- and three-body interactions



$$p_m^{\mathrm{2B}}(\boldsymbol{r}_1, Z_1, \boldsymbol{r}_2, Z_2) := \|\boldsymbol{r}_1 - \boldsymbol{r}_2\|^{-m}$$

$$p_{m_1,m_2,m_3}^{\mathrm{3B}}(\boldsymbol{r}_1, Z_1, \boldsymbol{r}_2, Z_2, \boldsymbol{r}_3, Z_3) := \frac{1}{\|\boldsymbol{r}_{12}\|^{m_1}\|\boldsymbol{r}_{13}\|^{m_2}\|\boldsymbol{r}_{23}\|^{m_3}} \cdot\theta(Z_1, Z_2, Z_3, \|\boldsymbol{r}_{12}\|, \|\boldsymbol{r}_{13}\|, \|\boldsymbol{r}_{23}\|)$$

Predicting atomization energy



K. Hansen, .., A. Tkatchenko, K.-R. Müller, , *J. Chem. Theory Comput.*, 9, (2013).
W. Pronobis, A. Tkatchenko, K.-R. Müller, *J. Chem. Theory Comput.*, 14, (2018).
O.A. von Lilenfeld, K.-R. Müller, A. Tkatchenko, *Nat. Rev. Chem.*, 4, (2020).

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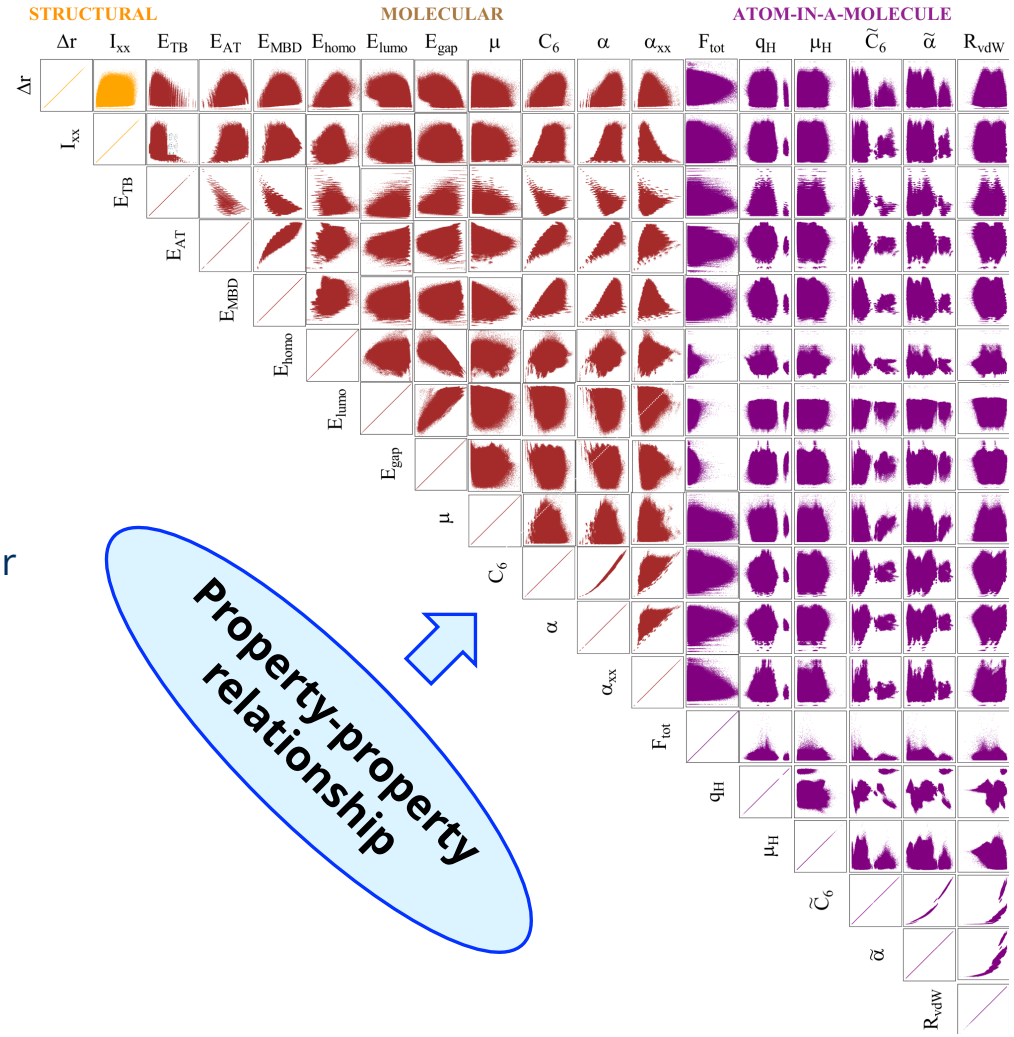
Defining novel QM descriptors

- Structural properties
  - Atomic positions
  - Moment of inertia tensor
- Molecular properties
  - PBE0 atomization energy
  - MBD dispersion energy
  - HOMO-LUMO gap
  - Dipole moment
  - Molecular polarizability
  - Molecular polarizability tensor
  - C_6 coefficient
- Atom-in-a-molecule properties
  - Total atomic forces
  - Hirshfeld charges
  - Hirshfeld dipole moment
  - Atomic polarizabilities
  - vdW radii



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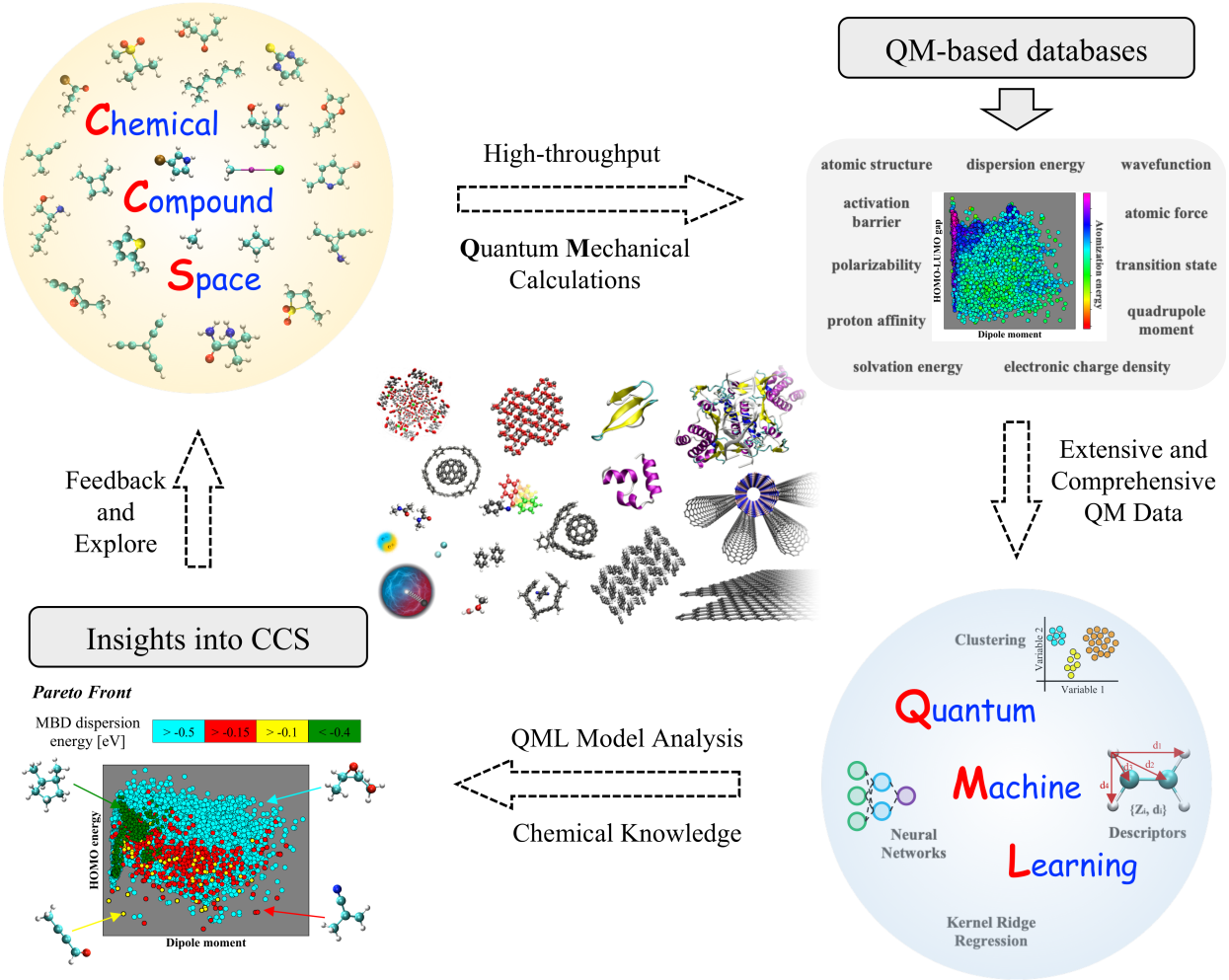
Machine learning for chemical discovery



A. Tkatchenko, *Nat. Commun.*, 11, 4125, (2020).

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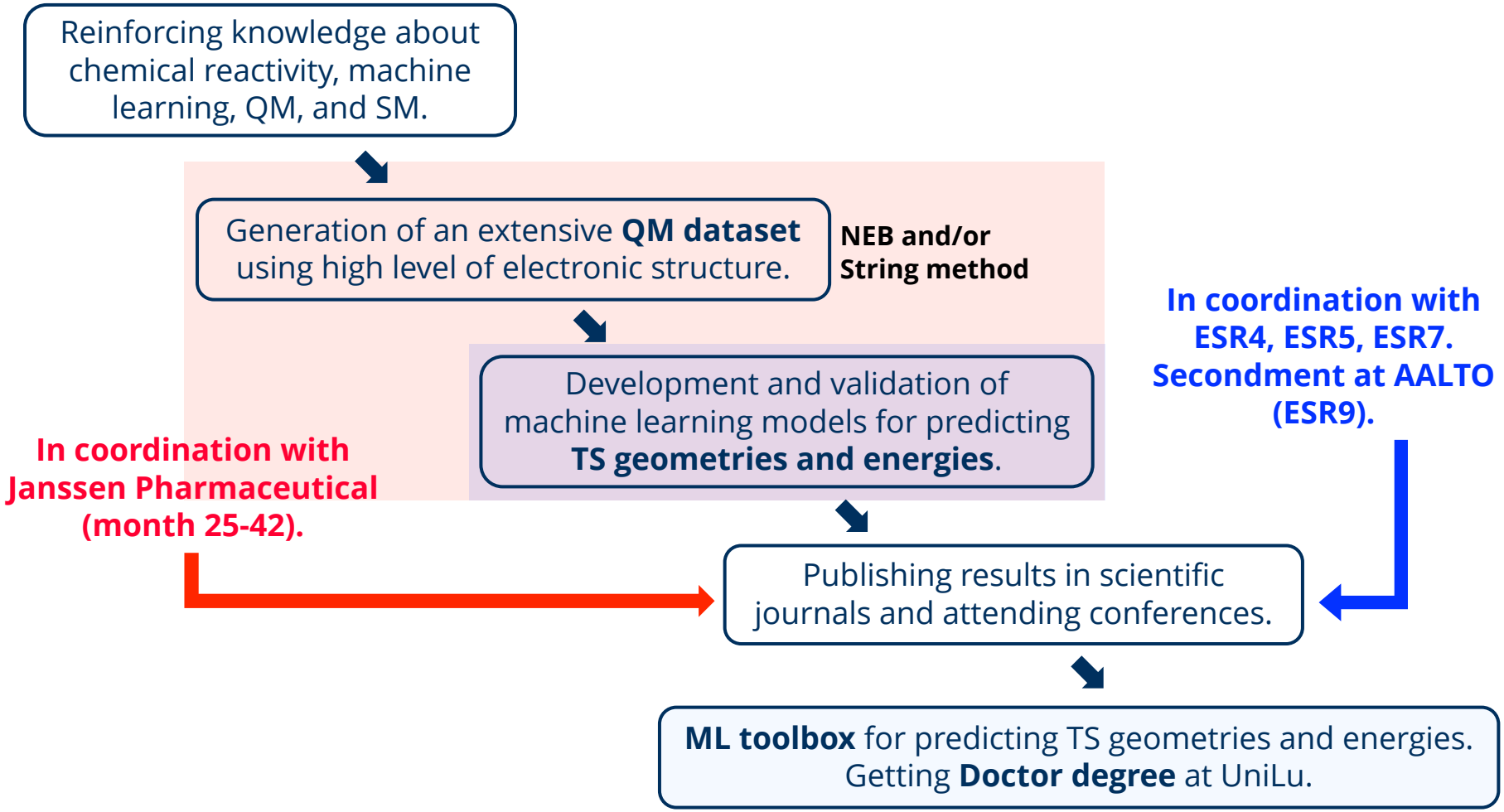
Work plan for the doctoral student



Many thanks for the attention.