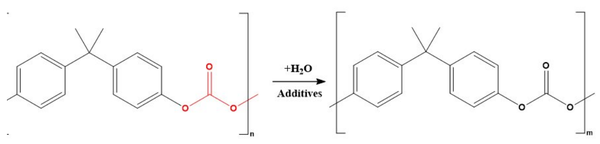
DRD APAC

What is quantum chemistry? What is it for?

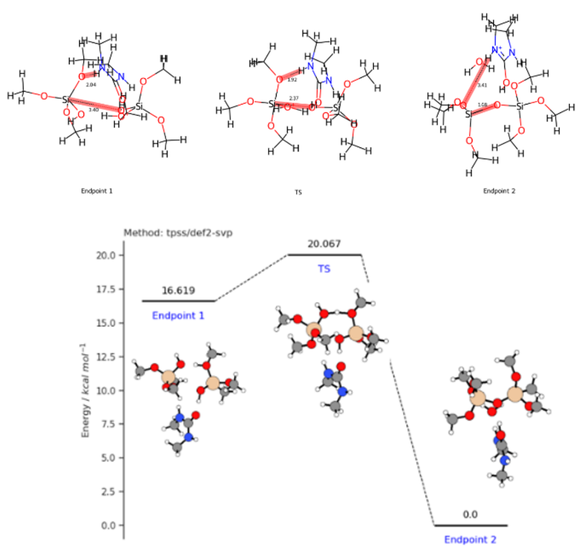
- ab-initio approaches to the calculation of the electronic structure and properties of molecules.
- Approximation methods: Hartree-Fock (HF), Configuration interaction (CI), Density Functional Theory (DFT), independent electron pair approximation, perturbation approach, one-particle green's function, etc.
- Reaction mechanism study (catalytic, surface), material properties (electronic, transport, solubility, etc), conformational study, inter/intra molecular interaction



Lactone/ester sodium salt in PC hydrolysis	Ea,ES [Kcal/mol]
Dialkyloxalate, 1, X=Me	≥ 26.1
Dialkyloxalate, 2, X= Na	≥ 34.7
Methylformiate	23.4
$H_2PO_4^-$	5.7
Na-citrate / citric acid	11.4 / 22.8
H_3PO_4(excess of free acid)	18.3

BPA based Hydrolysis Reaction Study

Bisphenol-A (BPA) based Polycarbonate(PC), hydrolysis test consists of more than thousand hours testing time. The additives from various sources may influence the hydrolysis performance of the Bisphenol-A (BPA) based Polycarbonate(PC). The project is intended to use QM determining the reaction kinetics of the hydrolysis process on ester bond in BPA. Considered additives are included base, acid, minerals, etc. By using the simulation results, we have identified the candidates which may enhance the anti-hydrolysis properties of the materials. This process could also potentially shorten the duration of the hydrolysis test, which is normally around 1000 hours



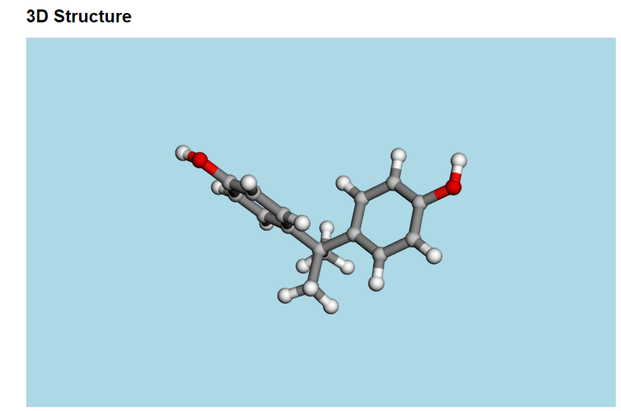
Silanol condensation study in L2 -Inorganic-organic hybrid CA

We have utilized DFT calculations to determine the reaction barrier of the dimerization of Silanols which are believed to be the primary cause of the storage problem of the mixture of L2-Inorganic-organic coating material. After screening various reaction conditions and the effects of other existing compounds on the condenstaion reaction, suggestions have been made about pH condition, which may help identify the optimum storage conditions.

QUANTUM CHEMISTRY IN COVESTRO

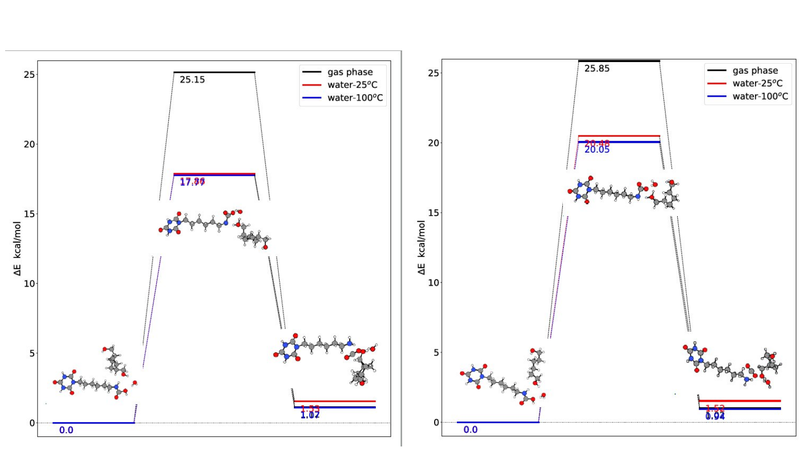
In-House Tools

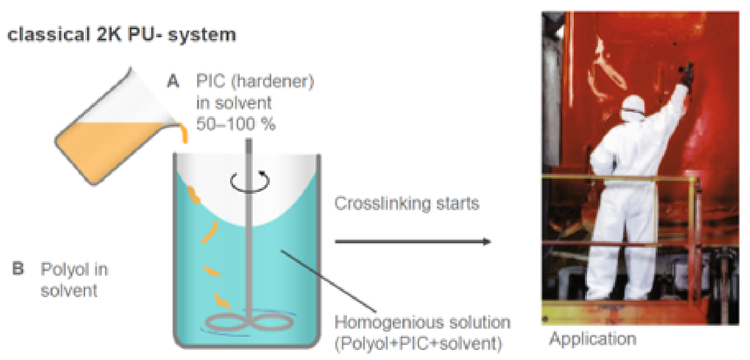
- NEB
- Berny optimization (Gaussian)
- Bayesian optimization
- TS-Toolkit
- QM calculator web-based platform



QM calculator web-based platform

A web application for quantum chemistry calculations which is designed to derive various properties such as total energy, HOMO-LUMO gap, dipole moment, IR-spectrum etc. It is an interface of a collection of different methods including developed ML models and quantum chemistry programs which can be rapidly accessed via web-based frontend. Ideal users are simulation experts and experimentalist who want to access quantum chemistry related information via common molecular name.





CO2 release step of model HDI trimer and 1,4-cyclohexandimetanol/1,6-hexanediol

The aliphatic isocyanate laboratory consistently focuses on enhancing BFFT (Blister-Free Film Thickness), a crucial performance metric for the 2K waterborne coating system. With the application of advanced multi-scale simulation techniques, the DRD team has actively supported our laboratory in understanding the impact of hardener recipes on the final application performance. QC simulations have effectively refuted potential interpretations of how specific diols significantly influence CO2 release by analyzing the kinetic barrier of reactions.