Faculty of Materials and Chemical Engineering
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ANTAL KERPELY DOCTORAL SCHOOL OF
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Thesis Booklet of the Doctoral Dissertation

entitled

Organocatalytic Urethane Synthesis – A Computational Study

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INTRODUCTION

The field of polymer science emerged to develop new materials for growing civil and military needs. It tends to be more interdisciplinary than most sciences, combining chemistry, chemical engineering, and other fields as well[1,2]. In 1937 one of the most special polymer types with versatile properties was discovered[3] **(Figure 1)**. This special type of polymer is polyurethane (PU), which was developed by Otto Bayer to compete with nylon[4,5]. Bayer's invention ranks among the most important breakthroughs in polymer science.
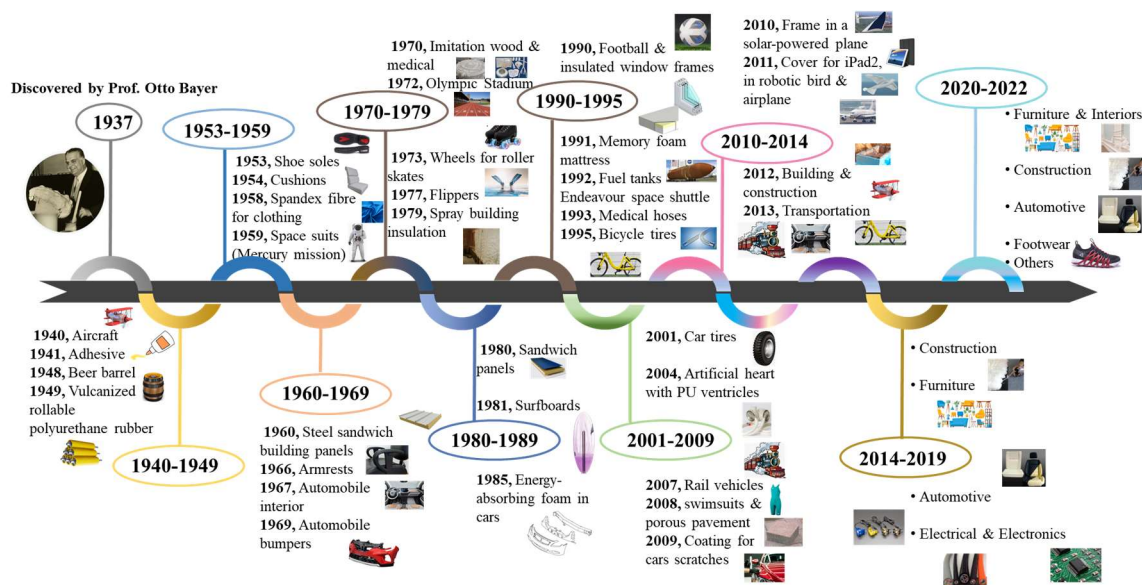

Figure 1. Timeline of major developments in the history of polyurethane.

Polyurethane is used in a large array of industries as flexible, and rigid foams, elastomers, and thermoplastic materials[6]. Most of the PU types are designed to make life more comfortable and products more durable[7,8]. Polyurethanes (PU) are a special group of heterochain polymers, formed by the reaction of isocyanate (NCO) and hydroxyl (OH) groups[9,10]. Isocyanate is a chemical that contains at least one isocyanate group (-N=C=O) in its structure. In PU synthesis two types of isocyanates, aromatic and aliphatic ones are used[11]. The other main raw materials in PU synthesis are polyols containing two or more hydroxyl groups[12]. Beside the effect of the chemical structure and the functionality of isocyanates and polyols on urethane formation[13], polyurethane synthesis can be finetuned by applying various additional compounds such as catalysts, chain extenders, crosslinkers, surfactants, and blowing agents[14]. In relation to PU synthesis, catalysts are often used to accelerate the reaction rate of polynucleophiles with isocyanate groups or to promote the trimerization of the isocyanate group to form cross-linked polymers. In the production of PU, the amount of applied catalysts is small, but their impact is significant[15]. Catalysts play an important role in the control and balance between the gelling and

blowing reactions. They help to accurately control the relative reaction rates of the isocyanate with both alcohol and water. The imbalance between these is one of the reason for the foam to collapse or the formation of inappropriate cells that can be closed or opened prematurely[16,17]. Polyurethane catalysts mainly include organic acids, organic bases (amine catalysts), and organo-tin (organometallic) compounds[18–21]. Organic acids are able to promote urethane formation under mild polymerization conditions and low catalyst loadings[22]. Amine catalysts applied in PU synthesis can be divided into aliphatic, cyclic, aromatic, alcohol, and ether amines[20],[23].

MOTIVATION OF THE DISSERTATION

The motivation of my work was to better understand urethane formation processes both with and without the presence of different organocatalysts by using computational chemistry tools.

METHODS

Different density functional methods were tested such as B3LYP[24], BHandHLYP[25], and ωB97X-D[26], in combination with the 6-31G(d)[27–29] basis set. However, only the BHandHLYP method was suitable to locate all the critical points on the potential energy surfaces (PES) of the studied catalytic processes. The effect of solvent (*e.g.* acetonitrile, MeCN, $\varepsilon_r = 35.688$) has also been considered by employing the SMD polarizable continuum model.

To further improve the accuracy of the results, the G3MP2BHandHLYP composite method[30–32] was applied and used in the discussion of the results. The G3MP2BHandHLYP composite method was not applicable in case of larger species (*e.g.*, 2,2-dimorpholinodiethylether (DMDEE)), because the computational cost of the calculations exceeded the available limit. Therefore, a quasi-G3MP2BHandHLYP (qG3MP2BHandHLYP) protocol was employed as it was described before[33].

Furthermore, to handle the thermodynamic properties of zwitterionic structures within the proposed mechanisms a correction which was previously successfully used in the literature to handle a similar system was employed[34].

NEW SCIENTIFIC RESULTS – THESIS

During my Ph.D. I studied the effect of organocatalysts on urethane formation using computational tools, and the following main conclusions are drawn as new scientific results:

1st Thesis

Method test has been carried out and a computational protocol applicable to the study of catalytic and catalyst-free urethane formation reactions has been selected. The protocol includes the G3MP2BHandHLYP composite method in combination with the SMD implicit solvation model. To keep the computational protocol as simple as possible, but finetune the energy of zwitterionic species, a correction has also been introduced and applied **(Figure 1T)**.
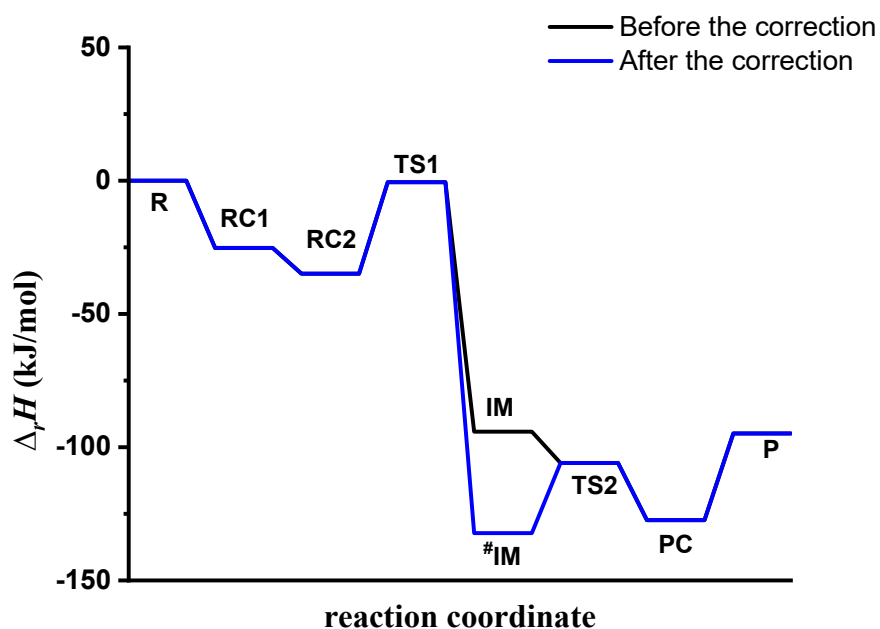
Figure 1T Relative enthalpy ($\Delta_r H$) profile of the phenyl isocyanate (PhNCO) and butan-1-ol (BuOH) reaction in the preseance of 4-methylmorpholine (catalyst) before (black line) and after the correction (blue line).

2nd Thesis

The catalyst-free reaction mechanism of phenyl isocyanate and alcohol (methanol (MeOH), and butan-1-ol (BuOH)) has been described by applying density functional theory and composite methods. It was found that the relative enthalpy difference in the barrier heights ($\Delta_r H_{[TSBuOH-TSMeOH]}$) when MeOH or BuOH are involved in the reaction with phenyl isocyanate is just 0.3 kJ/mol, which indicates that increasing the length of the aliphatic chain of the alcohol did not have a significant effect on urethane bond formation **(Figure 2T)**.
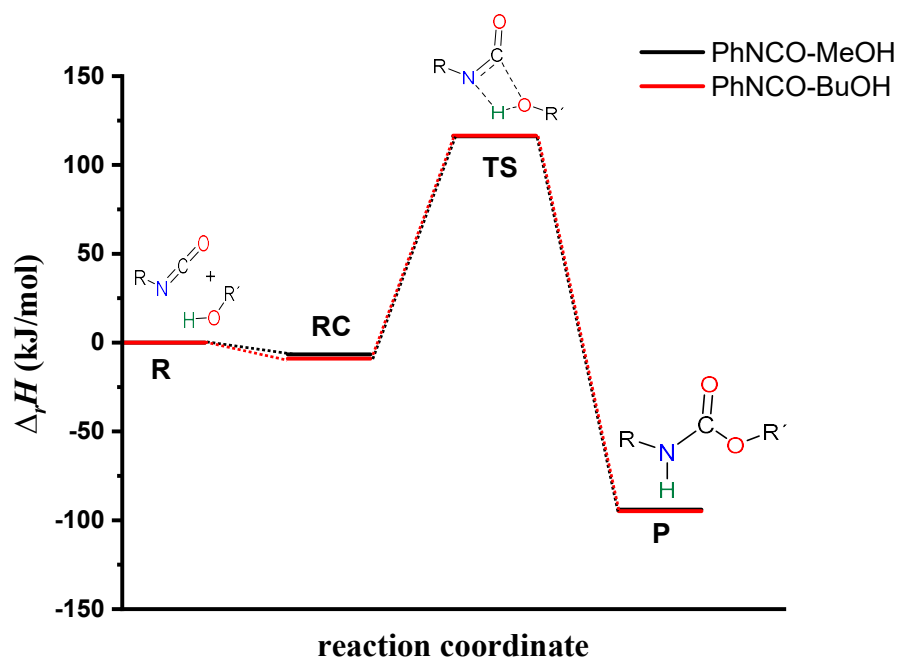

Figure 2T Relative enthalpy ($\Delta_r H$) profile of phenyl isocyanate (PhNCO) - methanol (MeOH) and PhNCO - butan-1-ol (BuOH) reactions, indicated with black and red lines, respectively. Calculated at the G3PMP2BHandHLYP theory level (298.15 K and 1 atm) in acetonitrile using the SMD implicit solvent model.

3rd Thesis

*A general mechanism for catalytic urethane formation in the presence of amine catalysts has been proposed and verified by using theoretical methods and literature data **(Figure 3T)**.* The mechanism was tested in the cases of 18 catalysts. The proposed reaction mechanism of amine catalysed urethane formation contains seven steps. It starts with the formation of an alcohol-catalyst complex (RC1), which is followed by the formation of an alcohol-catalyst-isocyanate trimolecular complex (RC2). After these steps, a proton transfer occurs between the alcohol and the amine group of the catalyst (TS1). This leads to the next step where the intermediate (IM) will be formed. Thereafter, the catalyst will return the proton through a transition state (TS2), and thus, a product complex is formed (PC). In the final step, the catalysts and the product will be separated (P).
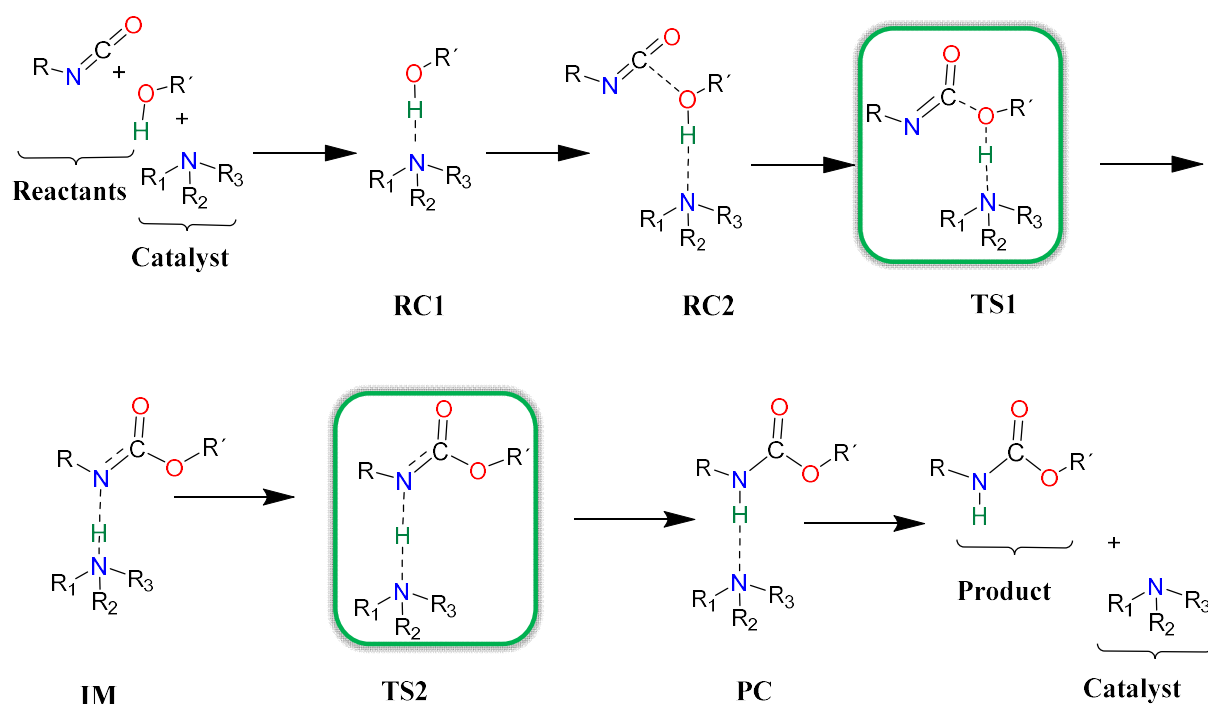

Figure 3T Schematic representation of the general amine -catalized urethane formation mechanism, where RC—reactant complex, TS—transition state, and PC—product complex.

4th Thesis

A general mechanism for catalytic urethane formation in the presence of acid catalysts has been proposed and studied using theoretical methods (Figure 4T). The proposed reaction mechanism of acid catalysed urethane formation contains five steps. First, a complex (RC1) between the alcohol and the catalyst is formed. Then, in the next step the isocyanate is added to the system, and RC2, a trimolecular complex is formed. After the complex formation, transition state (TS) develops and where a proton transfer between the alcohol and the catalyst, also between the N=C=O and catalyst occurs. Before the reaction completes, a product complex (PC) is forming, where the urethane bond is complete. In the final step, the catalysts and the product will be separated (P). The mechanism was tested in case of three different acid catalysts.
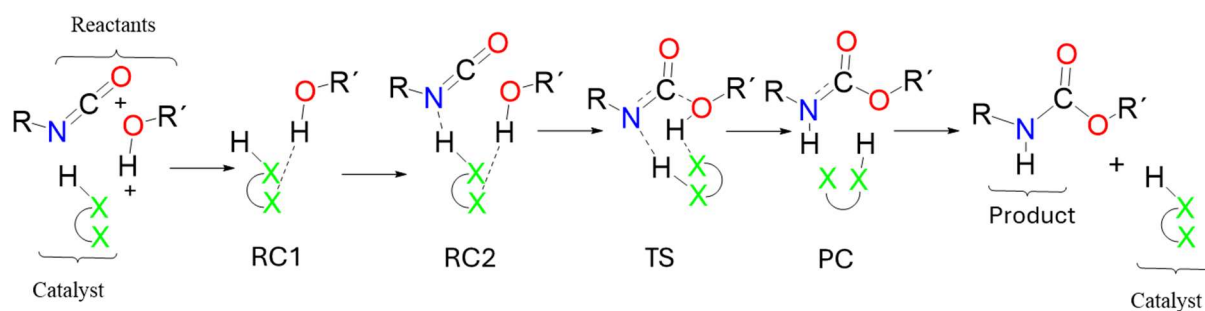

Figure 4T Schematic representation of the general organic acid-catalyzed urethane formation, where RC—reactant complex, TS—transition state, and PC—product complex.

5th Thesis

A new reaction mechanism was proposed for the stoichiometric reaction between 2-dimethylaminoethanol (DMEA) and phenyl isocyanate **(Figure 5T)**. By comparing the catalytic and stoichiometric processes, it was found that the catalytic process is more effective for urethane formation even if the difference in energy is not so high. Thus, DMEA can act as an effective catalyst and after some time, it can also react with free isocyanates and be built into the polymer chain which will reduce the volatile organic compound (VOC) content in the final product.
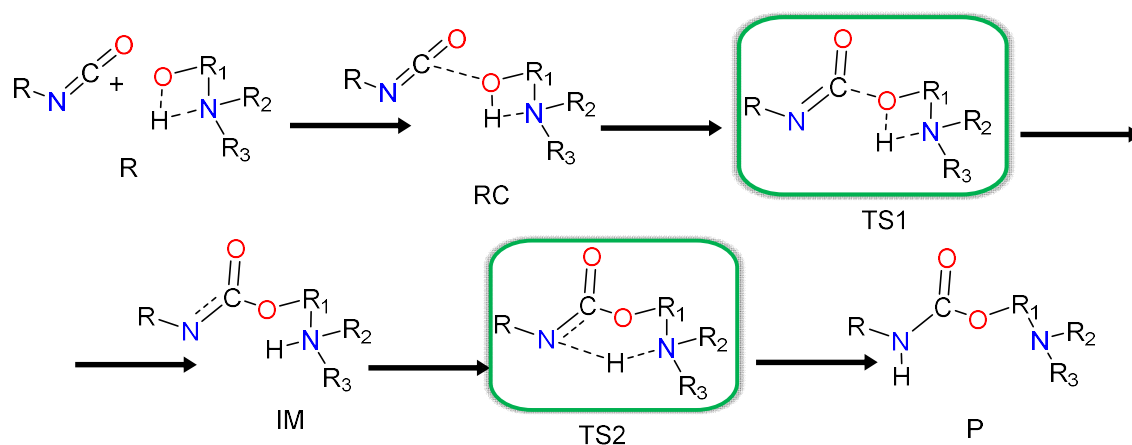
Figure 5T Schematic representation of the reaction mechanism of 2-dimethylaminoethanol (DMEA) - isocyanate stoichiometric reaction, where R—reactant, RC—reactant complex, TS—transition state, IM—intermediate, and PC—product complex.

SUMMARY

Polyurethanes are some of the most versatile and unique polymers used in the industry for manufacturing a wide variety of products. The synthesis of polyurethanes from diisocyanates and polyols under industrial conditions requires a catalyst or often a combination of catalysts, which can be regarded as the most important component of the reaction system besides the starting materials. Therefore, one of the main development trends in PU synthesis is finding improved catalysts. In this doctoral dissertation, urethane formation in catalyst-free and catalytic processes was studied using computational chemical tools, and the general formation mechanisms are proposed in the presence of amine and acid catalysts. The catalyst-free reaction mechanism of phenyl isocyanate and alcohol (methanol (MeOH), and butan-1-ol (BuOH)) has also been described. It was found that the relative enthalpy difference in the barrier heights ($\Delta_r H_{[\text{TSBuOH-TSMeOH}]}$) when MeOH or BuOH are involved in the reaction with phenyl isocyanate is just 0.3 kJ/mol, which indicates that increasing the length of the aliphatic chain of the alcohol did not have a significant effect on urethane bond formation.

Furthermore, the applicability of the proposed general amine catalysed urethane formation mechanism was tested and verified in the case of 18 catalyst. Additionally, the general mechanism for urethane formation in the presence of acid catalysts has also been tested and studied for three systems.

Some of the studied amine catalysts contain reactive functional groups (*e.g.* OH) and thus, these species can act as stoichiometric reactants with isocyanates which will lead to the formation of urethane bonds. Therefore, a stoichiometric reaction was proposed when 2-dimethylaminoethanol (DMEA) reacts with phenyl isocyanate. It was found that DMEA can act as an effective catalyst and after some time, it can also react with free isocyanates and be built into the polymer chain which will reduce the volatile organic compound (VOC) content in the final product. Taking into account the environmental impact of VOC reduction, these results can be employed in the design of more effective and safer catalysts for polyurethane synthesis.

It can be stated, that through this doctoral dissertation, a deeper understanding of the effect of catalysts on urethane formation is achieved. Meanwhile, the computed and measured thermodynamic properties were in good agreement with each other, which proves the validity of the proposed mechanisms and verifies the method selection as well.

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LIST OF PUBLICATIONS

Publications Related to the Subject of the Dissertation

1. **Hadeer Q. Waleed**, Marcell Csécsi, Rachid Hadjadj, Ravikumar Thangaraj, Dániel Pecsmány, Michael Owen, Milán Szőri, Zsolt Fejes, Béla Viskolcz, and Béla Fiser, ″Computational study of catalytic urethane formation,″ *Polymers*, **2022**, 14, 8, DOI: 10.3390/polym14010008. (Q1; IF=5.0)
   Number of Independent Citations: 5

2. **Hadeer Q. Waleed,** Dániel Pecsmány, Marcell Csécsi, László Farkas, Béla Viskolcz, Zsolt Fejes, and Béla Fiser, ″Experimental and theoretical study of cyclic amine catalysed urethane formation,″ *Polymers*, **2022**, 14, 2859, DOI: 10.3390/polym14142859. (Q1; IF=5.0)
   Number of Independent Citations: 1

3. **Hadeer Q. Waleed**, Marcell Csécsi, Vivien Konyhás, Zsanett R. Boros, Béla Viskolcz, Zsolt Fejes, and Béla Fiser, ″Aliphatic tertiary amine catalysed urethane formation – a combined experimental and theoretical study,″ *Phys. Chem. Chem. Phys*., **2022**, 24, 20538, DOI: 10.1039/d2cp00728b. (Q1; IF= 3.676)
   Number of Independent Citations: 2

4. **Hadeer Q. Waleed**, Rachid Hadjadj, Béla Viskolcz, and Béla Fiser, ″Effect of morpholine, and 4-methylmorpholine on urethane formation: a computational study,″ *Sci Rep*., **2023**, 13, 17950, DOI: 10.1038/s41598-023-44492-x. (D1; IF= 4.6)
   Number of Independent Citations: 0

5. **Hadeer Q. Waleed**, Béla Viskolcz, Zsolt Fejes, and Béla Fiser, ″Urethane formation in the presence of 2,2-dimorpholinodiethylether (DMDEE) and 1,4-dimethylpiperazine (DMP) – A combined experimental and theoretical study,″ *Computational and Theoretical Chemistry,* **2023***, 1221, 114045, DOI: 10.1016/j.comptc.2023.114045. (Q3; IF= 2.8)
   Number of Independent Citations: 3

6. **Hadeer Q. Waleed**, Rachid Hadjadj, Béla Viskolcz, and Béla Fiser, ″Stoichiometric reaction and catalytic effect of 2-dimethylaminoethanol in urethane formation,″ *Phys. Chem. Chem. Phys,* **2024**, 26, 7103-7108, DOI:10.1039/D3CP05800J (Q1; IF= 3.676)
   Number of Independent Citations: 0

Further Publications

1. **Hadeer Q. Waleed**, Marcell Csécsi, Rachid Hadjadj, Ravikumar Thangaraj, Michael Owen, Milán Szőri, Zsolt Fejes, Béla Viskolcz, and Béla Fiser, ″The catalytic effect of DBU on urethane formation – A computational study,″ *Materials Science and Engineering*, **2021**, 46, 70–77, doi:org/10.32974/mse.2021.008.

2. **Hadeer Q. Waleed**, Fejes Zsolt, Viskolcz Béla, Fiser Béla, ″Experimental and theoretical study of urethane formation in the presence of amine catalyst,″ *Symposium on Polyurethane Innovation - SPI 2022, Conference publications,* **2022**, 203, 28-35.

3. **Hadeer Q. Waleed**, Béla Fiser, ″Polyurethane synthesis and classification - A mini-review,″ *Doktorandusz Almanach,* **2022**, 1, 116-127.

4. Mallouhi Julie, **Hadeer Q. Waleed**, Szőri-Dorogházi Emma, Owen Michael, Fiser Béla, ″Molecular dynamics study of the closed conformations of Candida rugosa lipase 2 (CRL),″ *Symposium on Polyurethane Innovation - SPI 2022, Conference Publications*, **2022**, 203, 82-90.

5. **Hadeer Q. Waleed**, Béla Fiser, ″The catalytic effect of 1,4-diazabicyclo[2.2.2]octane (DABCO) on urethane formation - A computational study,″ *Doktorandusz Almanach*, **2023**, 1, 91-97.

6. **Hadeer Q. Waleed**, Edina Reizer, Béla Viskolcz, Béla Fiser, ″A computational study of the catalytic effect on urethane formation,″ *Symposium on Polyurethane Innovation – SPI 2023 - Conference Publications*, **2023**, 230, 19-27.

7. **Hadeer Q. Waleed**, Dalal K. Thbayh, Amal Zarrami, Julie Mallouhi, Pecsmány Dániel, Reizer Edina, Rachid Hadjadj, Fiser Béla, ″Hogyan tervezhetünk jobb polimereket szuperszámítógépek segítségével?,″ *HPC ECHO, Tudománytól Innovációig*, 2021, 10-12.

8. **Hadeer Q. Waleed**, Dalal K. Thbayh, Amal Zarrami, Julie Mallouhi, Pecsmány Dániel, Reizer Edina, Rachid Hadjadj, Fiser Béla, ″How can we design better polymers with supercomputers?,″ *HPC ECHO, From Science to Innovation*, 2021, 10-12.

9. Rachid Hadjadj, Imre G. Csizmadia, **Hadeer Q. Waleed**, Dalal K. Thbayh, Béla Viskolcz, Béla Fiser, ″Monoethanolamine assisted CO2 hydrogenation to methanol – A computational study,″ Molecular Catalysis, Vol. 559, pp.114091, 2024. DOI: 10.1016/j.mcat.2024.114091. (Q2; IF= 4.6).

Presentations and posters

1. A Miskolci Egyetem Kémiai Intézetének (KI, MAK, ME) és a MAB Elméleti és Fizikai Kémiai Munkabizottságának közös rendezvénye

   Oral presentation/Online/Miskolc, Hungary, 2021.05.11.

   A Computational Study of Urethane Formation.

2. Symposium on Polyurethane Innovation SPI 2021

   Oral presentation/Online/Miskolc, Hungary, 2021.08.24.

   Computational Study of Urethane Formation in the Presence of Catalysts.

3. 37. Borsodi Vegyipari Nap

   Oral presentation/Online/Miskolc, Hungary, 2021.11.17.

   Catalytic Effect of Amine Catalysts on Urethane Formation - A Computational Study.

4. 25th Spring Wind Conference

   Poster presentation/Pécs, Hungary, 2022.06-08.05.

   Catalytic Effect of Tertiary Amine on Urethane Formation.

5. Symposium on Polyurethane Innovation SPI 2022

   Oral presentation/Miskolc, Hungary, 2022.11.11.

   Experimental and Theoretical Study of Urethane Formation in the Presence of Amine Catalyst.

6. 10th Visegrad Symposium on Biomolecular Interactions

   Poster presentation/Nove Hrady, Czech Republic, 2022.06.16.

   Experimental and Theoretical Study of Tertiary Amine Catalysed Urethane Formation.

7. Hungarian Science Day

   Oral presentation/Miskolc, Hungary, 2022.11.09.

   Polyurethane Catalysis by Tertiary Amines - A Combined Theoretical and Experimental Study.

8. 26th Spring Wind Conference

   Oral presentation/Miskolc, Hungary, 2022.05-07.05.

   Experimental and Theoretical Study of Urethane Formation in the Presence of Tertiary Amine Catalyst.

9. 11th Visegrad Symposium on Biomolecular Interactions

   Poster presentation/Szidonia Castle, Hungary, 2023.20-23.06.

Amine Catalysed Urethane Formation – A Combined Experimental and Theoretical Study.

10. 10th Doctoral Symposium on chemistry

Poster presentation/Lodz, Poland, 2023.18-19.05.

Cyclic Amine Catalysed Urethane Formation- A Combined Experimental and Theoretical Study.

11. Symposium on Polyurethane Innovation SPI 2023

Oral presentation/Miskolc, Hungary, 2023.08.24.

A Computational Study of the Catalytic Effect on Urethane Formation.

12. Basics & Application of Computational Chemistry in Action (BACCA), Erasmus+ Blended Intensive Programme, virtual session

Oral presentation/Online, 2024.04.04

Organocatalytic Urethane Synthesis– A Computational Study.

Scientometrics

- Total number of publications: 15
- Total number of first author publications: 13
- Total number of second author publications: 2
- Total number of Q1 publications: 5
- Total number of Q2 publications: 1
- Total number of Q3 publications: 1
- Total number of independent citations: 11
- H index: 4