**Sustainable Water Management**

**Doctoral Programme (Water4All)**

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| **Title of the PhD Project** | The development of sustainable and novel green membranes for water treatment |
| **Acronym** | GreenMemB |
| **Research Fields of the Project** | Membrane Science and Technology; Material Science and Engineering; Chemical Engineering |
| **Keywords** | Green solvents, green membrane, water treatment, cellulose, deep eutectic solvent |
| **Host Institution, Department and Campus Location** | İzmir Institute of Technology, Chemical Engineering Department |
| **PhD Awarding Institution and Graduate Programme** | İzmir Institute of Technology, Chemical Engineering Department |
| **Name and Affiliation of Main Supervisor** | Prof. Dr. Sacide Alsoy ALTINKAYA |
| **Name and Affiliation of Co-Supervisors** | Assoc. Prof. Dr. Sadiye VELİOĞLU |
| **Research Environment and Infrastructure** | IZTECH has all the facilities for membrane preparation, testing and characterization. These facilities include membrane casting device, filtration set-up, surface charge, contact angle measurement devices, surface roughness and morphological characterization tools.<br><br>The MEM-CES laboratory at the Institute of Nanotechnology, Gebze Technical University (GTU) has three high-capacity workstations available for molecular simulation. Two of these workstations have 16 cores, while the third has 64 cores. Additionally, the lab is eligible to use the TRUBA cluster system, which offers high GPU and memory allocation for simulations. |
| **Scientific Context of the Project** | This study will be structured into three parts. The first part will utilize molecular dynamics simulations (MD) to comprehend the factors influencing cellulose dissolution in various combinations of deep eutectic solvents (DES) and molecular solvents. Specifically, the investigation will focus on understanding the dependence of cellulose dissolution on the molecular structures of both DES and molecular solvents. |

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| | In the second part, experimental studies will be conducted to validate the accuracy of the simulation results and identify optimal solvents for membrane preparation. The optimization process will be based on the levels of cellulose dissolution and the viscosity of the solvents.<br><br>The third part will involve the development of new high-flux ultrafiltration membranes with a low fouling tendency. The impact of the designed solvent's structure on the membrane's morphology will be investigated. Additionally, the relationship between the morphological features of the membrane and its filtration performance will be explored through detailed characterizations. These characterizations will encompass viscosity measurements for the polymer solution, cloud point measurements, thickness, porosity, pore size, contact angle of the membranes, FTIR, XPS, DSC, SEM, and AFM analyses. The antifouling property of the developed membranes will be assessed using model foulants. |
| **Brief Workplan** | Academic year of 2024-2025: Screening of DES and molecular solvent combinations with molecular simulations<br>Academic year of 2025-2026: Membrane development and morphological characterization<br>Academic year of 2026-2027: Membrane filtration tests |
| **Innovative Aspects of the Project** | The membrane technology cannot be considered environmentally friendly unless the fabrication process of the membrane itself is sustainable. This necessitates the substitution of oil-derived polymers with bio-based or renewable polymer materials and the preference for non-toxic solvents over conventional toxic ones. Cellulose is an excellent starting material for membrane preparation since it is one of the most abundant and biodegradable materials on Earth. However, the strong intermolecular hydrogen bonding and crystalline nature of cellulose makes its dissolution difficult. Various solvents including N,N-dimethylacetamide/ lithium chloride (DMAc/LiCl), N-methylmorpholine-N oxide (NMMO) mono-hydrate, ionic liquids (ILs), and NaOH/urea aqueous solvents were used for dissolving cellulose. Regrettably, these solvents rely on harsh chemicals, demand substantial energy for processing, and/or generate byproducts that are not entirely environmentally benign. Thus, finding environmentally friendly solvents for cellulose dissolution remains an ongoing challenge to facilitate the development of green membranes from this abundant source.In recent years, deep eutectic solvents (DESs) have received considerable attention. These solvents are composed of two or more components linked by hydrogen bonding networks, resulting in significantly lower melting temperatures compared to the individual components. Various combinations of these components offer a broad spectrum of compositions tailored to specific applications. Despite numerous tested combinations, cellulose dissolution by DESs has not surpassed 10 wt%. This study aims to develop a new class of green solvents capable of dissolving cellulose under mild conditions. This will be achieved by combining different DESs with molecular solvents at various ratios. The project's novelty lies in utilizing both experimental and theoretical approaches to understand biopolymer-solvent interactions for efficient cellulose dissolution. This generic approach aims to create an entirely new class of green solvents capable of dissolving cellulose under mild |

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| | conditions, facilitating the development of cellulose membranes that meet sustainable and green membrane criteria. |
| **Training Opportunities of the Project** | In CNR-ITM, PhD students will have access to the laboratory equipment including membrane casting machine, micro-, ultra- and nanofiltration rigs and advanced characterisation and analytical equipment (scanning electron microscopy, contact angle, mechanical test machine, FT-IR and porometer). The students will have also full access to open internet and full free access to scientific journals. The annual meeting organized by the Institute (ITM Seminar Days) can be used by the PhD students as a platform to present their work. |
| **Interdisciplinary Aspects** | This project integrates three interdisciplinary fields: membrane science and technology, chemical engineering, and material science and engineering. The expertise required for membrane development, surface modification, and characterization—focusing on filtration capacity and morphological features such as pore size distribution and surface charge—necessitates a background in membrane science. Additionally, proficiency in both theoretical and experimental tools for membrane characterization will require an approach rooted in both Chemical Engineering and Material Science and Engineering. |
| **Intersectoral Mobility**<br><br>☐ **Short Visit**<br><br>☐ **Secondment** | TBD |
| **International Academic Secondment** | Host Supervisor: Dr. Alberto Figoli<br><br>Host Institution: Institute on Membrane Technology (CNR-ITM) National Research Council of Italy<br><br>Duration: 6 months<br><br>Estimated Time of Mobility: 2025 |

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| **Main Supervisor:** | |
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| **Brief CV** | **Prof. Dr. Sacide ALSOY ALTINKAYA**<br>**E-mail:** sacidealsoy@iyte.edu.tr<br>**Academic Degrees**<br>Ph.D. Chemical Engineering, The Pennsylvania State University, USA 1998<br>M.Sc. Chemical Engineering, Ege University, Türkiye 1993<br>B.Sc. Chemical Engineering, Ege University, Türkiye 1991<br>**Professional Networks**<br>Google Scholar:<br>https://scholar.google.com/citations?user=KkNm_8UAAAAJ&hl=en<br>Research Gate:<br>https://www.researchgate.net/profile/Sacide-Altinkaya<br>Scopus:<br>https://www.scopus.com/authid/detail.uri?authorId=6603259612<br>ORCID:<br>https://orcid.org/0000-0002-7049-7425 |
| **Co-supervisor:** | |
| **Brief CV** | **Assoc. Prof. Dr. Sadiye VELİOĞLU**<br>**E-mail:** sadiyevelioglu@gtu.edu.tr<br>**Academic Degrees**<br>Ph.D. Material Science and Eng., Istanbul Tech. University, Türkiye 2015<br>M.Sc. Material Science and Eng., Istanbul Tech. University, Türkiye 2008<br>B.Sc. Chemical Engineering, Istanbul Technical University, Türkiye 2006<br>**Professional Networks**<br>Google Scholar:<br>https://scholar.google.com.sg/citations?user=mNTLPsUAAAAJ&hl=en |

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