EPFL

SEMINAR SERIES

HIGHLIGHTS IN ENERGY RESEARCH

02.04.2020, 16:00 - 17:00, EPFL Valais, 4th floor, TSEUZIER room

High-Throughput Computational Screening of MOFs for CO2 Separation

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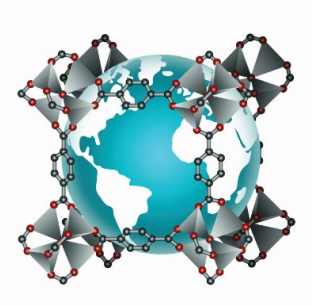
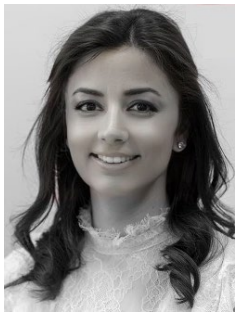
Host : Prof. Berend Smit

We have witnessed the quick growth of a new generation nanoporous materials named as metal organic frameworks (MOFs) in the last decade. MOFs have exceptional physical, chemical and structural properties such as low densities, large surface areas and high porosities which make them promising materials for a large variety of applications, mainly for CO_2 separation. The number of MOFs has been increasing very rapidly and experimental identification of materials exhibiting high CO_2 separation potential is simply impractical. High-throughput computational screening studies in which several thousands of MOFs are evaluated to identify the best candidates for a target gas separation is crucial in directing experimental efforts to the most useful materials. In this talk, we will show how molecular simulations were used to screen the MOF database to identify the best materials for CO_2 separation from flue gas (CO_2/N_2) and landfill gas (CO_2/CH_4) in addition to CO_2/H_2 and CH_4/H_2 separations. We first validated molecular simulations by comparing the simulated CO_2 uptakes, CO_2/N_2, CO_2/CH_4, and CO_2/H_2 selectivities of various types of MOFs with the available experimental data and then computed several adsorbent evaluation metrics such as selectivity, working capacity, and regenerability of MOFs. The top performing MOFs for each gas separation were identified based on the combination of these metrics. We will also discuss the relations between structural properties of MOFs and their separation performances to provide structure-property relationships that can serve as a map for experimental synthesis of new MOFs with better performances. These results will accelerate the design and development of novel materials for efficient CO_2 capture and separation.



Metal Organic Frameworks (MOFs) will save the world.



Bio: Seda Keskin is a professor at the Department of Chemical and Biological Engineering at Koç University and she acts as the Associate Dean for Research at the College of Engineering. She received her undergraduate and MSc. degrees from the Department of Chemical Engineering, Bogazici University in 2004 and 2006, respectively. She completed her PhD at the School of Chemical and Biomolecular Engineering, Georgia Institute of Technology in 2009. Her PhD thesis on the atomistic modeling of nanoporous membranes received the Sigma Xi Best Doctoral Dissertation Award and Chemical and Biomolecular Engineering Outstanding PhD Thesis Award. Her research expertise is in atomically-detailed simulations of new generation nanoporous materials for energy applications. She was the recipient of L'Oreal Young Women in Science Award, Turkish Academy of Sciences Distinguished Young Scientist Award, The Science Academy Young Scientists Award, TUBITAK Encouragement Award, Parlar Foundation Research Incentive Award, FABED Outstanding Achievement Award and Koç University Outstanding Faculty Award. She received the European Research Council's ERC-Starting Grant in 2017, and she was recently elected to the Global Young Academy as the representative of Turkey in engineering.