VRIJE UNIVERSITEIT BRUSSEL

The faculty of Engineering of the Vrije Universiteit Brussel invites you to attend the public defense leading to the degree of

DOCTOR OF ENGINEERING SCIENCES

of **Mahsa Najafi Lahiji**

The public defense will take place on **Thursday 4th September 2025 at 1 pm** in room **D.2.01** (Building D, VUB Main Campus)

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SEPARATION OF LIGHT OLEFINS FROM PARAFFINS USING OLEFIN-SELECTIVE ADSORBENTS VIA KINETIC AND EQUILIBRIUM DISCRIMINATION

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Abstract of the PhD research

light olefins such as ethene and propene are essential building blocks for the petrochemical industry. Their large-scale production through cracking yields mixtures with paraffinic impurities (ethane and propane), which must be removed to meet downstream requirements. Today, polymer-grade olefins are produced mainly by cryogenic distillation which is an extremely energy-intensive process that contributes heavily to CO_2 emissions because of the nearly identical physicochemical properties of olefin/paraffin pairs. Developing alternative, energy-efficient separation methods is therefore a scientific and industrial priority, with adsorption on porous materials emerging as a promising pathway.

For equilibrium-based separation, the study focuses on metal–organic frameworks (MOFs), examining their adsorption behavior, selectivity, and uptake capacity. Special attention is given to the influence of surface functionalities and open metal sites, which provide valuable insights into the molecular mechanisms that enable efficient separation. In another approach, titanosilicate ETS materials with finely tuned pore sizes were evaluated for their potential in kinetic separations. Through systematic equilibrium and diffusion studies, as well as binary mixture experiments in a dynamic system, the work reveals how the interplay between competitive adsorption and molecular diffusion governs separation performance.

Together, these findings advance the fundamental understanding of adsorptive separation mechanisms and highlight that a systematic evaluation of adsorption behavior and mixture separation performance is essential for identifying the potential of porous adsorbents in developing practical and energy-efficient light olefin/paraffin separation processes.