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Doctoral dissertation evaluation report

Author of the thesis:	Jakub Halamek
Title of the thesis:	Adsorptive Separation of Small Molecules on Zeolitic Materials
Thesis evaluator:	prof. David Kubička, Ph.D., University of Chemistry and Technology Prague, Czech Republic

The doctoral thesis of Jakub Halamek explores in a meticulous and systematic way the separation of carbon dioxide and methane, and of mixtures of gaseous hydrocarbons over zeolites. The work focuses on the identification and elucidation of key structural / topological parameters. The thesis is based on five articles in renowned journals out of which 3 were already published. He is the first author one of the published articles and two that are either submitted or being finalized. Nonetheless, his contribution to each of the articles / manuscripts should be explicitly stated in the thesis.

The dissertation thesis is of very high scientific relevance and quality as reflected by the top journals in which the research findings were published. The quality of the dissertation can be compared to the quality of theses at top European universities I had the privilege to review. From the formal point of view, the thesis is well organized, easy to read with a minimum number of typos using good English. Nevertheless, a couple of things could have been improved. In particular, a list of abbreviations and symbols used is missing, the use of abbreviated verb forms, such as “isn’t”, is not appropriate in scientific English and SI units should be used (various units of pressure are used throughout the thesis).

For the defense of the thesis I would like to raise several points:

1. Please, can you give examples of processes where each type of the industrial adsorption regeneration (as reported on 11) is being used.

2. CO separation from syngas is mentioned as a commercial application of π-complexation. Can you give a specific example of this since syngas is generally the targeted intermediate stream and the CO to H_2 ratio is typically adjusted water gas shift reaction?
3. On page 15, activated carbon (AC) is given as an example of an adsorbent with a non-polar surface. Does AC really have a non-polar surface?
4. FER has similar pore sizes as the studied PCR material. Was FER investigated as a commercially produced benchmark? If not – why? If yes – what were the results?
5. You discuss the complexity of C4 fraction separation on page 31. Would you know how isobutetene is efficiently and selectively separated from the mixture of C4 hydrocarbons in the industry?
6. Fig. 15 – I assume that Si-CHA does not possess any protons and would expect that the heat of adsorption would be independent of the coverage. But it is not the case. This is attributed to the adsorbate-adsorbate interactions. However, in case of Al-CHA the values of heat of adsorption drop below the benchmark value of Si-CHA at higher coverages. Why? Why in this case do not the adsorbate-adsorbate interactions result in an increase in the heat of adsorption like in the case of Si-CHA?
7. Fig. 16 – Looking at the Si/M ratios and the schematic representation, M is replacing Si only in every second or even third MR. Hence, why signal "splitting" in the spectra is observed only for B-CHA, but not Ga-CHA and Al-CHA?
8. The larger CO_2 uptake of Na-exchanged samples is attributed to better accessibility of cationic sites (page 49). Why should be the Na^+ sites be better accessible than the Li^+ sites?
9. The best performance of CHA is attributed to an interplay of high uptake, high selectivity, low regeneration costs and cheap synthesis (page 52). I agree that these are all important, but it is not clear what they mean as they are discussed only in a relative manner while the conclusions should be quantitative. It would be interesting to learn what is "high uptake" (e.g. larger than XX mmol/g), “high selectivity” (e.g. larger than XY), “low regeneration costs” (e.g. less than XZ euro) and “cheap synthesis” (e.g. less than YZ euro).
10. Insufficient quality of IPC-9 has been hypothesized based on the experimental results. This looks as an important feedback for material synthesis to me. Was it possible to have prepared another batch (a better one) of the same material?
11. With respect to the exceptional separation activity of PCR material, it is not clear to me if the high concentration of defects (silanol groups) is really important for the exceptional adsorption behavior or if this is caused by the foreign species / impurities?

In summary, even though I have raised several points for discussion, the doctoral dissertation of Jakub Halamek is of top quality and I strongly recommend the dissertation for public defense.

Prof. David Kubička, Ph.D.