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Poster abstract

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Title: Theoretical study of aldol condensations on UiO-66 and UiO-66-NH_2

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Summary (max 200 words)**:**

Recently, metal-organic framework (MOF) compounds which are made up of inorganic and organic moieties have developed into an important new class of crystalline porous materials [1]. MOFs contain many metal sites, which might be catalytically active. This implies that MOFs have the potential to replace homogenous catalysts in important industrial applications [2]. Notwithstanding the catalytic activity of some of them- it is not always clear what the active sites are and how the reactions are catalyzed. Lately, the UiO-66-NH_2 has successfully been applied experimentally for the synthesis of jasminaldehyde from benzaldehyde and heptanal [3]. To fully understand the mechanism of jasminaldehyde condensation on such open active Zr-sites, we applied molecular modeling techniques on extended cluster as well as on periodic model of the UiO-66-X materials. On an extended cluster, the most plausible condensation reaction mechanism was found, showing that benzaldehyde and heptanal are adsorbed and activated on adjacent Zr sites. On the UiO-66-NH_2 model, there should be also an alternative reaction route, where one of the two aldehydes is activated on the amino group, explaining the higher selectivity of the UiO-66-NH_2 compared to the UiO-66 [3]. Deeper insight into these complex mechanisms allows us to explain the selectivity and activity on the UiO-66 type materials.

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[2] Czaja, A. U., Trukhan, N. and Muller, U., Chem. Soc. Rev. 38 (2009) 1284.
[3] Vermoortele, F., Ameloot, R., Vimont, A., Serre, C., De Vos, D., Chemical Communications 47 (2011) 1521.