

Synthesis and Functionalization of Ordered Mesoporous Silica: Improved Catalyst Carrier Materials through Pore Size Control and Metal Incorporation

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Studying confinement effects in molecular heterogeneous catalysis requires access to mesoporous support materials with well-defined, yet variable, pore sizes. Although ordered mesoporous silica (OMS) - prime candidates for this task - have been studied extensively since the pioneering work of Kresge et al. [1], these materials are not readily available. We demonstrate that direct liquid crystal templating at high surfactant concentrations produces OMS with Gaussian pore size distributions [2], and that this method enables precise tuning of pore sizes between 2.5 and 20 nm when using high-molar mass block copolymers [3].

To enhance the catalytic role of the support material, we study the incorporation of various metal atoms into the OMS, potentially creating Lewis acid sites that offer additional substrate coordination. We will demonstrate that our labor and material efficient synthesis method results in well-defined ordered mesoporous metallosilicates (OM²S) with high metal loadings and open pores. Furthermore, we will elucidate how synthesis conditions and pore sizes influence the number and strength of the Lewis and Brønsted acid sites. Finally, we will discuss achieving an atomistic understanding of the presented OMS and OM²S through a combined experimental and theoretical approach.

[1] C.T. Kresge, M.E. Leonowicz, W.J. Roth, J.C. Vartuli, and J.S. Beck, *Nature*, 1992 **359**, 710–712, DOI: 10.1038/359710a0.

[2] J.R. Bruckner, J. Bauhof, J. Gebhardt, A.-K. Beurer, Y. Traa, and F. Giesselmann, *J. Phys. Chem. B* 2021, **125**, 3197–3207, DOI: 10.1021/acs.jpccb.0c11005.

[3] C. Vogler, S. Naumann, and J.R. Bruckner, *Mol. Syst. Des. Eng.* 2022, *7*, 1318–1326, DOI: 10.1039/D2ME00107A.