

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Corrected OCM dataset employed in the current study.

File Name: Supplementary Data 2

Description: Element property table with basic physical and chemical properties of chemical elements and their compounds as assembled from literature and own measurements.

File Name: Supplementary Data 3

Description: Table that lists for each catalyst compound in the OCM dataset the assigned property descriptors.

File Name: Supplementary Data 4

Description: Table that lists for each catalyst in the OCM dataset the assigned property groups that were obtained via application of the sorting rules.

File Name: Supplementary Data 5

Description: Table that provides for the final model a list of catalyst compositions (i.e. cation combinations) contained in each property group.