



## PRESS-RELEASE

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### THE HYSTRAM CONSORTIUM HAS IDENTIFIED THE PROSPECTIVE CATALYSTS TO ENHANCE THEIR DESIGN FOR AMMONIA PRODUCTION

The HySTrAm project is working to develop innovative solutions to facilitate the transformation of hydrogen into ammonia thereby contributing to the decarbonisation of the energy sector. As an initial step, Kemijski inštitut (KI) has established a list of prospective catalysts for ammonia production based on literature search, educated guess and simulations.

Based on modelling and literature data, Kemijski inštitut has performed a list of prospective catalyst materials which will be used as starting point and benchmark in designing better catalysts for ammonia production. Throughout the process, KI have used density functional theory calculations and kinetic simulations to replicate different catalysts and **the analysis results identified ruthenium (Ru)-based structures with dopants and iron (Fe) as the most promising catalysts for improvement.**

According to the collected data, the ruthenium-based structures include flat surfaces, steps, kinks and nanoparticles. The researchers identified alkali and earth alkaline metals to be useful to the doping mechanisms. Additionally, the upcoming research will use cobalt (Co) and molybdenum (Mo) based formulations and alloys as benchmark catalyst models.

Kemijski inštitut stressed that “*designing a catalyst is an arduous process relying on extensive simulations*”. After establishing a list of catalyst materials for further scrutiny, the project will be able to focus on a more targeted search during the lifespan of the project.



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