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v Ljubljani

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*in kemijsko tehnologijo*

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**VABILO NA PREDAVANJE  
V OKVIRU DOKTORSKEGA ŠTUDIJA  
KEMIJSKE ZNANOSTI**

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z naslovom:

**Catalyst by Design**

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*Vljudno vabljeni!*

**Abstract:**

Utilizing hydrogen in place of fossil fuels is a promising clean energy alternative. Designing catalysts that are able to generate hydrogen, convert it into consumer-friendly energy resources, and upgrade chemicals to meet the needs of industry is an important pillar of the hydrogen economy. It is a major challenge in catalysis to uncover structure-performance relationships that drive the design and optimization of high-performance/low cost catalysts. When one considers the number of potential elemental combinations for catalysts and then includes variables, such as particle size and elemental stoichiometry, the number of possibilities is daunting. There are also significant challenges facing the synthetic chemist, who is tasked with making and characterizing such complex architectures. Indeed, a way of substantially narrowing the field is essential. In this work, we introduce a novel and effective approach that combines computational prediction, experimental verification using a well-defined nano-model produced by scanning probe block copolymer lithography, and finally production of high-performance catalysts in bulk as a powerful tool for discovering and designing catalysts for energy conversion and storage.

**References**

- (1) Huang, L.L.; Chen, P.; Liu, M.H.; Fu, X.B.; Gordiichuk, P.; Yu, Y.N.; Wolverton, C.; Kang, Y.J.\*; Mirkin, C.A.\* *Proc. Natl. Acad. Sci. USA*, 2018, 115 (15), 3764-3769
- (2) Kang, Y.J.; Yang P.D.; Markovic, N.M.; Stamenkovic, V.R. *Nano Today*, 2016, 11 (5), 587-600