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Cation-Site Disordered Cu3PdN Nanoparticles for Hydrogen Evolution Electrocatalysis

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¬¬Transition metal nitrides (TMNs) are emerging as a promising class of materials for application in optoelectronics as well as energy conversion and storage, but they remain rather unexplored, mainly due to a lack of mechanistic understanding of their synthetic pathways. Here we demonstrate a one-pot synthesis, which yields 3 nm phase-pure Cu3PdN nanoparticles after the reaction of Cu methoxide and Pd acetylacetonate in benzylamine for 5 minutes at 140℃. We reveal the structure of the initial complexes and their conversion to Cu¬3PdN by in situ x-ray absorption spectroscopy measurements and elucidate nucleation and growth of the nitride nanocrystals by in situ total x-ray scattering measurements. Interestingly, extended x-ray absorption fine structure double-edge refinement reveals the presence of short-range cation-site disorder in the anti-perovskite structure of Cu3PdN, which has not been observed before in the Cu3PdN system. Additionally, the synthesized Cu3PdN nanoparticles are tested for the electrocatalytic hydrogen evolution reaction revealing an overpotential as low as η10 = 212 ± 11 mV measured at 10 mA/cm2.

Author: KOPULA KESAVAN, Jagadesh (Universität Hamburg)

Co-authors: KÖPPEN, Andrea (Universität Hamburg); DIPPEL, Ann-Christin (Deutsches Elektronen-Synchrotron (DESY)); KOZIEJ, Dorota (Universität Hamburg); CADDEO, Francesco (Universität Hamburg); Dr NOEI, Heshmat (Center for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany); KLEMEYER, Lars (Universität Hamburg); BELGARDT, Lian (Universität Hamburg); GUMUS AKCAALAN, Melike (UniversitÃ¤t Hamburg); Dr MATHON, Olivierq (ESRF); HAROUNA-MAYER, Sani (Universität Hamburg); GRÖNE, Tjark Leon Raphael (Universität Hamburg)

Presenter: KOPULA KESAVAN, Jagadesh (Universität Hamburg)

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