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Structure and functionality of a prospective (Pt, Ru)/MgO nanocatalyst RYSZARD BUCZKO, Oak Ridge National Laboratory, ALBINA BORISEVICH, Oak Ridge National Laboratory, RICHARD ADAMS, University of South Carolina, MICHAEL AMIRIDIS, University of South Carolina, STEPHEN PENNYCOOK, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University — The atomic structure of metal nanoparticles in the prospective catalyst (Pt, Ru)/MgO was imaged by Z-contrast scanning transmission electron microscopy. On the MgO (110) surface we find regular monolayer-like particles; all atoms show uniform intensity in the image and are likely to be Pt because of the large atomic number. Density functional theory calculations have been used to determine the structure of possible particles. We find that regular monolayer-like structures can be formed, with Pt bonded to surface oxygen. The Pt particles are loosely connected to the substrate in agreement with microscopic observations. The influence of surface defects on cluster structure and mobility will be analyzed, and the implications for the catalytic activity of the (Pt, Ru)/MgO system will be discussed.

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