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Atomic-scale study of the Rh/γ-alumina catalytic system SHUPING ZHUO, School of Chem. Eng., Shandong Univ. of Tech., YIPING PENG, Condensed Matter Sci. Div., ORNL, STEPHEN PENNYCOOK, Condensed Matter Sci. Div., ORNL, KARL SOHLBERG, Chem. Dept., Drexel Univ. — Prerequisite to the non-empirical design and refinement of improved heterogeneous catalysts is the identification of the atomic-scale structure and properties of the catalytically active sites. We report an investigation of the Rh/γ-alumina system, which is representative of many common heterogeneous catalysts that consist of transition metals dispersed on a high surface area support. Previous atomic-resolution Z-contrast STEM observations have shown Rh-containing "rafts" on the (100) exposure. This finding is surprising given that the preferred exposure of γ-alumina is (110). First-principles density functional studies and image simulations suggest that these Rh-containing structures consist of the high-pressure rhodium sesquioxide (II) phase growing on the surface. The high pressure phase of rhodium sesquioxide and γ-alumina (100) exposure yield improved interface match over the regular rhodium sesquioxide phase and γ-alumina (110) exposure.

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