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題目(和文)	アンモニア合成及び分解における触媒担体上のルテニウムとアニオンの相互作用の役割
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論 文 要 約

論文題目 Thesis Title	Role of Ru-anion interaction on the support surface in synthesis and decomposition of ammonia （アンモニア合成及び分解における触媒担体上のルテニウムとアニオンの相互作用の役割）

要約

This thesis clarifies the role of interactions of Ru and anion constituting the support at interfaces in NH_3 synthesis and decomposition by experiments and density functional theory calculations. The primary conclusions obtained are two. First, the covalent bonding between Ru and various anions (Si^{4-}, N^{3-}, O^{2-}, F^{-}) of the support materials works effectively to keep the Ru particle sizes to several nanometers. Second, key mechanisms of NH_3 synthesis on Ru/Ca_2NH and decomposition on $Ru/C12A7:e^{-}$ are revealed as follows; i) anionic electrons are transferred into loaded Ru, which promotes N-N bond cleavage and formation. ii) $H^{\delta-}$ at the interface, which is more stable than on Ru surface, can prevent the hydrogen poisoning of Ru surface. iii) N-H bond formation is promoted by the reaction of $H^{\delta-}$ and N adatom at the interface.