Supporting Information

Fischer-Tropsch Product Selectivity Modulation via FeRh Nanocluster Composition Design

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Figure S1. The optimized geometric structures of the FeₙRh₁₃₋ₙ nanoclusters. The green and purple atoms represent rhodium and iron, respectively.
Figure S2. Optimized adsorption geometries of CO molecule on the Fe$_n$Rh$_{13-n}$ (n=1, 2, 6, 11, and 12) nanoclusters.
Figure S3. Optimized adsorption geometries of HCO + H and COH + H on the Fe₉Rh₁₃₋ₙ (n=1, 2, 6, 11, and 12) clusters.
Figure S4. Optimized adsorption geometries of CH$_2$O + 2H and CH$_3$O + H on the Fe$_n$Rh$_{13-n}$ (n=1, 2, 6, 11, and 12) nanoclusters.