SUPPORTING INFORMATION for

Mechanisms of Alumina Growth via Atomic Layer Deposition on Nickel Oxide and Metallic Nickel Surfaces

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Figure S1. Reactant, intermediate images, and product for the TMA molecule decomposition path to DMA molecule plus CH3 radical group adsorbed on each one of the surfaces evaluated. No intermediate structures for TMA decomposition are shown for Ni(211) surface as the dissociation reaction occurs in a spontaneous manner from the TMA adsorption, and the most favorable geometry for the coupled DMA plus CH_3 radical adsorbed is equivalent with the one obtained from the TMA adsorption.



Figure S2. Reactant, intermediate images, and product for the DMA molecule decomposition path to MA molecule plus CH3 radical group adsorbed on each one of the surfaces evaluated



Figure S3. Reactant, intermediate images, and product for the MA molecule decomposition path to Al atom plus CH3 radical group adsorbed on each one of the surfaces evaluated.