Abstract Submitted
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Student Excellence Award Finalist: Computational study on the formation of Nickel hexafluoroacetylacetonate complexes Ni(hfac)$_2$ on a rough NiO surface during thermal atomic layer etching (ALE) Processes ABDULRAHMAN BASHER, Osaka University, MARJAN KRSTIC, Karlsruhe Institute of Technology (KIT), MICHIRO ISOBE, TOMOKO ITO, Osaka University, KARIN FINK, Karlsruhe Institute of Technology (KIT), MASATO KIUCHI, National Institute of Advanced Industrial Science and Technology (AIST), KAZUHIRO KARAHASHI, Osaka University, TAKAE TAKEUCHI, Nara Women's University, WOLFGANG WENZEL, Karlsruhe Institute of Technology (KIT), SATOSHI HAMAGUCHI, Osaka University — Thermal ALE by the formation of volatile organic metal complexes is expected to establish damageless and atomically controlled metal etching processes for nano-scale devices. For example, hexafluoroacetylacetone (hfacH) as an organic gas has proved its efficiency in etching magnetic metals at an elevated surface temperature. In a previous work, we demonstrated using first-principles quantum mechanical (QM) simulations how hfacH molecules are adsorbed and decomposed on a metallic nickel (Ni) surface while they can be adsorbed without decomposition on an oxidized nickel (NiO) surface. The goal of this study is to show how nickel hexafluoroacetylacetonate Ni(hfac)$_2$ is formed after hfacH molecues are adsorbed on a NiO surface. We have used Gaussian 09 and Turbomole codes to evaluate the interaction of hfacH molecules with flat and non-flat NiO surfaces to understand the conditions on which Ni atoms are removed from the surface by the formation of Ni(hfac)$_2$.

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