

Abstract Submitted
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CO₂ activation on TiO₂-supported Cu₅ and Ni₅ nanoclusters: Effect of plasma-induced surface charges¹ AMIN JAFARZADEH, ANNE-MIE BOGAERTS, ERIK C. NEYTS, Research group PLASMANT, Department of Chemistry, University of Antwerp, Universiteitsplein 1, B-2610 Antwerp, Belgium — Surface charging is an important factor in many plasma-surface interactions and in particular in plasma catalysis. In this study, we investigated the effect of excess electrons induced by plasma on the adsorption properties of CO₂ on titania-supported Cu₅ and Ni₅ clusters using spin polarized and dispersion corrected density functional theory. In addition, the effect of excess electrons on the deposition of Ni and Cu nanoclusters as well as on CO₂ adsorption on a pristine anatase TiO₂ (101) slab was studied. Our results indicate that CO₂ binds more strongly with a negatively charged surface. Increasing the surface charge density leads to a pronounced increase of the adsorption energy. Additionally, we also employed DFT+U calculations for cross-checking the results while accounting for the strong on-site Coulomb interactions, and the same trends are found.

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Amin Jafarzadeh
Univ of Antwerp

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