Short Communication

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Archives in Chemistry

2022
Vol 3. No. 2

Selecting the Reaction Path in On-Surface Synthesis through the Electron Chemical Potential in Graphene

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Abstract

The organometallic on-surface synthesis of the eight-membered sp2 carbon-based ring cyclooctatetraene (C8H8, Cot) with the neighboring rare-earth elements ytterbium and thulium yields fundamentally different products for the two lanthanides, when conducted on graphene (Gr) close to the charge neutrality point. Sandwich-molecular YbCot wires of more than 500 Å length being composed of an alternating sequence of Yb atoms and upright-standing Cot molecules result from the on-surface synthesis with Yb. In contrast, repulsively interacting TmCot dots consisting of a single Cot molecule and a single Tm atom result from the on-surface synthesis with Tm. While the YbCot wires are bound through van der Waals interactions to the substrate, the dots are chemisorbed to Gr via the Tm atoms being more electropositive compared to Yb atoms. When the electron chemical potential in Gr is substantially raised (n-doping) through backside doping from an intercalation layer, the reaction product in the synthesis with Tm can be tuned to TmCot sandwich-molecular wires rather than TmCot dots. By use of density functional theory, it is found that the reduced electronegativity of Gr upon n-doping weakens the binding as well as the charge transfer between the reaction intermediate TmCot dot and Gr. Thus, the assembly of the TmCot dots to long TmCot sandwich-molecular wires becomes energetically favorable. It is thereby demonstrated that the electron chemical potential in Gr can be used as a control parameter in an organometallic on-surface synthesis to tune the outcome of a reaction.

Received Date: 20 June, 2022 **Accepted Date:** 23 June, 2022 **Published Date:** 30 June, 2022

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