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Boudouard reaction under graphene cover on Ni(111)

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Ni is known to be a catalyst for the Boudouad reaction
$CO+CO \rightarrow CO2 + C$
which is favored by high pressure and thus escaped so far direct investigation under operando conditions. We report here on a Near Ambient Pressure XPS study performed at Soleil Synchrotron using the Tempo Beamline.
A bare Ni(111) sample has been exposed to CO at a pressure PCO~2 mbar. Graphene growth occurred already at 550 K [1], a temperature significantly lower than the one (670 K) at which growth of graphene by segregation of dissolved carbon occurs.
It has recently been shown [2] that the space between graphene layer and the substrate may act as a nano-reactor cavity where the activation barrier for CO oxidation is effectively reduced. We show here that this is the case also for the Boudouard reaction.
Exposing single layer graphene on Ni(111) to CO at 3.7 mbar, CO intercalates under the layer causing its detachment from the substrate. The so-obtained high local CO coverage under graphene cover enables the formation of CO2 via the Boudouard reaction catalyzed by the Ni(111) surface already at 340 K [3]. The carbon produced by the reaction is used to transform residual carbide into graphene. Moreover, under such conditions a chemisorbed CO species forms above the graphene film, thus paving the use of supported graphene for catalysis.
We also investigated the effect of the presence of vacancies obtained by low energy ion bombardment.
We find that CO intercalates at a rate which is comparable to the one observed in absence of defects and reacts via the Boudouard reaction producing additional carbon atoms and CO2.
While the former attach to the graphene layer and extend it over areas previously covered by carbide, the CO2 molecules bind to the graphene vacancies thus mending the defects. The so-formed complexes give rise to a peak at 533.4 eV which persists upon evacuating the vacuum chamber at room temperature and which we assign to a covalently bonded species containing C and O [4].

References
[1] R. Davì et al. Chem. Phys. Lett. 774, 138596 (2021)
[2] Q. Fu and X. Bao, Chem. Soc. Rev. 46, 1847 (2017)
[3] R. Davì et al, Appl. Surf. Sci. 599, 154065 (2022)
[4] R. Davì et al, submitted

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