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L-V | Carbon2Polymers: CO Conversion to Polycarbonates

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The aim of subproject L-V is to investigate the reaction of CO gas from a steel mill with Cl_2 for producing polycarbonates via phosgene as a key intermediate (Fig. 1). We investigate the interaction of Cl_2 with commercial activated carbons at different temperature via tracking formed gaseous products to draw structure-activity relationships. In close cooperation, the solvent-free phosgenation of phenol and life cycle assessment test is carried out at Covestro and RWTH Aachen, respectively.

EXPERIMENTAL APPROACH

Cl_2 activation is a crucial step for phosgenation. The interaction must not be too strong, otherwise, Cl_2 will deactivate the carbon (Fig. 2a). [1] By measuring the amount of Cl_2 adsorbed/desorbed on carbon at a temperature in a temperature programmed desorption, the reversibility and the nature of Cl_2 interaction with carbon are examined. Fig. 2b shows the set-up to evaluate the activated carbon's Cl_2 adsorption capacity since those parameters give important hints for catalytic performance. [2]

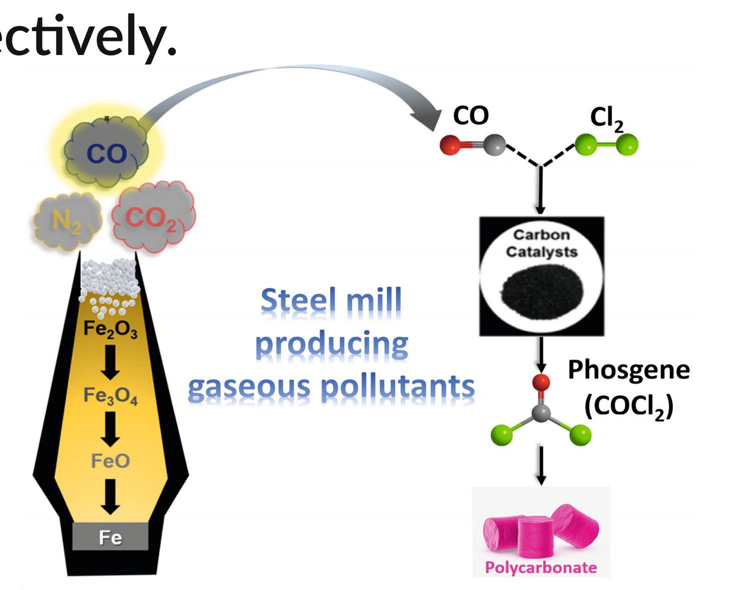

Fig. 1: Steel mill exhaust CO gas conversion to polycarbonate.

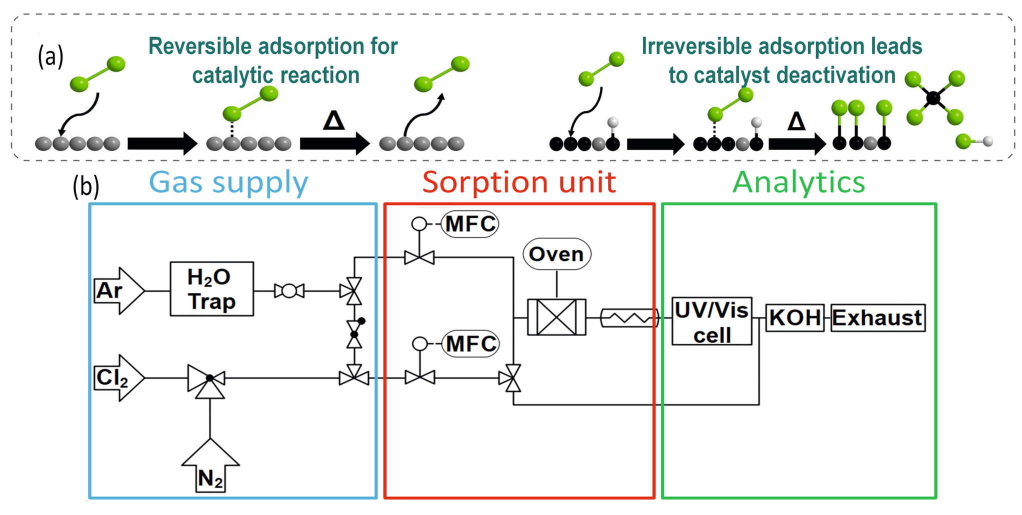

Fig. 2: (a) Scheme for reversible and irreversible Cl_2 adsorption on graphitic (left) and non-graphitic (right) carbon. (b) Set-up for Cl_2 interaction analysis. [3]

ACTIVITY/STABILITY TESTING OF ACT. CARBON

The Cl_2 adsorption/desorption experiment is carried out in tubular bed reactors over activated carbons (A-D). Fig. 3a shows the concentration of Cl_2 gas adsorbed at RT and desorbed at a higher temperature on Cat A. Compared to other carbons, Cat A exhibits a higher amount of Cl_2 adsorption/desorption, along with stable Cl_2 desorption over 3 cycles at RT (Fig. 3b,c). At higher temperature, the adsorbed Cl_2 decreases over cycle test, and desorbed Cl_2 is negligible (Fig. 3d). The lack of balance between the adsorbed and desorbed Cl_2 suggests the loss of Cl_2 gas in the side reactions, hence, deactivating the catalysts.

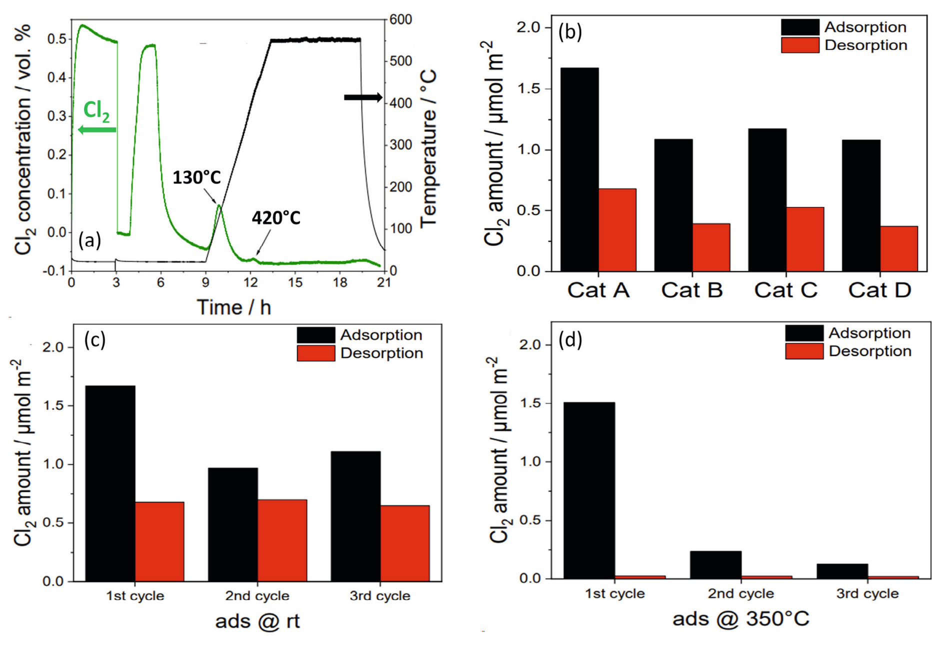

Fig. 3: (a) Cl_2 concentration during adsorption/desorption at RT on Cat A. (b) Amount of Cl_2 adsorbed/desorbed at RT on Cat A, B, C and D. Cycling test at (c) RT and (d) 350 °C on Cat A. [3]

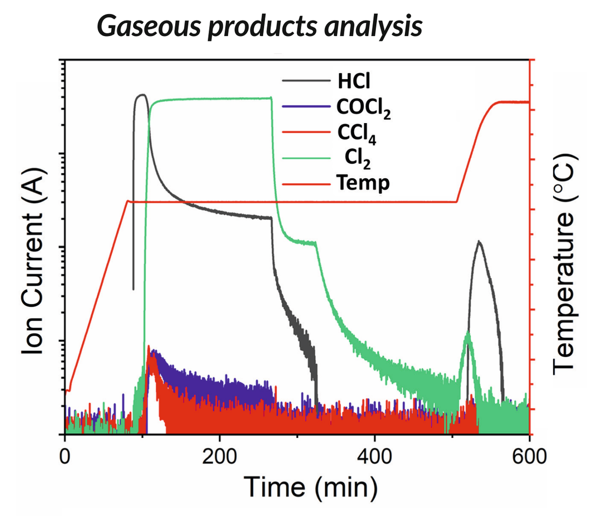

Fig. 4: Gases evolved during Cl_2 experiment.

WORK PROGRESS AND OUTLOOK FOR PHASE II

(i) Gaseous side products analysis using quadrupole mass analyzer produced during Cl_2 adsorption exp. on activated carbon (Fig. 4).

(ii) In situ Raman spectroscopy to investigate the changes in the carbon structure under the Cl_2 atmosphere at a particular temperature (Fig. 5).

References
[1] G. Centi, K. Barbera, S. Perathoner, N. K. Gupta, E. E. Ember, J. A. Lercher, ChemCatChem 2015, 7, 3036–3046.
[2] A. Bähr, G.-h. Moon, J. Diedenhoven, J. Kiecherer, E. Barth, H, Tüysüz, Chem. Ing. Tech. 2018, 90, 1513–1519.
[3] A. Bahr. Design of Nanostructured Carbon-Based Materials for Thermo- and Electrocatalytic Applications, 2021, Ph.D. thesis.

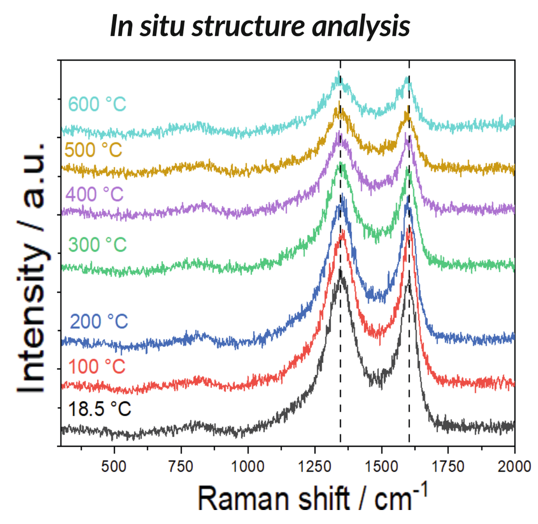

Fig. 5: Carbon structure change during Cl_2 experiment.

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