Oxygen functional groups responsible for the oxidative dehydrogenation of ethylbenzene to styrene over activated carbon fibres.

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During the styrene production reaction by oxidative dehydrogenation catalized by carbon, a continuous Polymer Organic Deposit (POD) takes place. This POD is known to be active in the aforementioned reaction and its presence increases the catalytic activity of some catalysts, for instance Al_2O_3. POD consists of a polyaromatic structure with a high proportion of oxygen groups on the edge of the rings. It is speculated that these oxygen groups (phenol and carbonyl) together with the aromatic rings are the active phase. Ethylbenzene can be adsorbed on the aromatic structure and stabilized by π-stacking interactions between the ring of the ethylbenzene and the rings of the POD. After this situation, oxygen groups are close to the ethyl group and the reaction can occur. The reaction takes place through the carbonyl/phenol and styrene/ethylbenzene redox couples. The results obtained by quasi-in-situ XPS-UPS show an important increase in the amount of surface oxygen during the reaction. This oxygen seems to be associated with oxygen groups belonging to the POD. The most remarkable result is the fact that the amount of both oxygen groups (carbonyl and phenol) in O_{1s} region, increases with reaction time and when the activity is increased (increasing the temperature or decreasing the flow). It can be concluded that carbonyl and phenol groups are involved in the oxidative dehydrogenation of ethylbenzene towards styrene.

Acknowledgement: J.A.M.-A. thanks Universidad de Alicante for the PhD Thesis fellowship. The authors thank MCYT the financial support (Project MAT 2000-06215).