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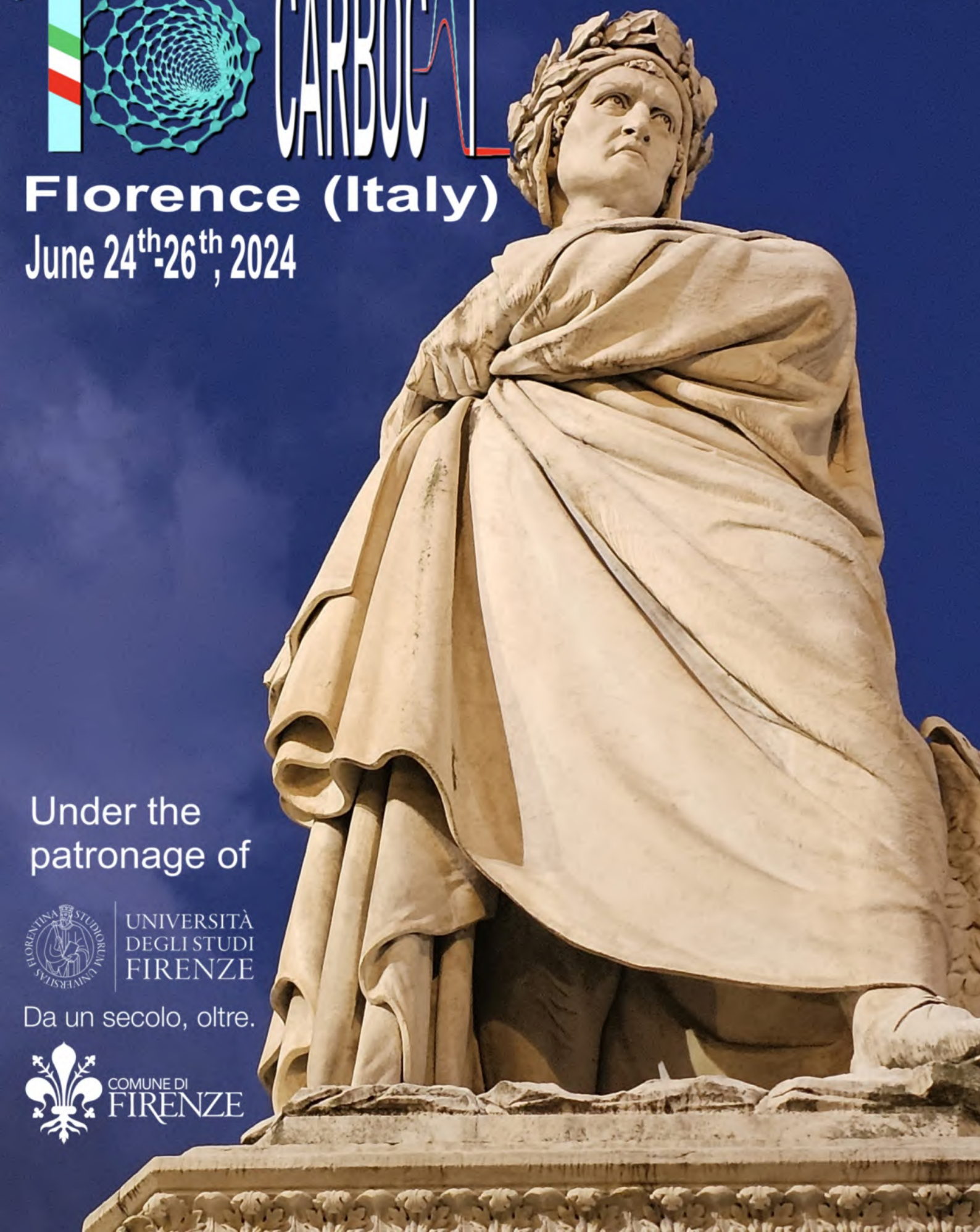

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BOOK of ABSTRACTS

OC05

NEW EVIDENCE ON THE ROLE OF CARBONYLS AS ACTIVE CENTERS FOR THE OXYGEN REDUCTION REACTION

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Besides carbon, oxygen is often the most abundant element within carbon materials. However, despite the extensive research efforts on carbon-based electrocatalysts for an oxygen reduction reaction (ORR), the role of oxygen functional groups in the ORR has rarely been studied without an important contribution of other properties (*e.g.*, crystallinity, porosity, and presence of other heteroatoms).[1,2] This study aims at bridging that knowledge gap, by conducting a systematic investigation on possible correlations between oxygen surface groups (carboxylic anhydrides, phenols, carbonyls, quinones, lactones, pyrones, and chromenes) and the ORR performances of a metal-free carbon catalyst in an alkaline medium. Graphite oxide was synthesized and thermally reduced at different temperatures (in the range 400 – 800 ºC) to promote the selective removal of oxygen surface groups. By enabling the synthesis of partially reduced graphene oxide samples with similar textural properties and crystalline structure, yet with different types and amounts of oxygen functional groups, our experimental results revealed a positive relationship between carbonyl groups and the ORR performance. The experimental results, combined with molecular modeling through density functional theory calculations, shed light on the previously overlooked role of oxygen functional groups in the ORR, opening a window of opportunity to advance the design of metal-free carbon electrocatalysts for this application.

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