



**CONGRESSO CONGIUNTO
SEZIONI CALABRIA E SICILIA**



**Università della Calabria, 1 e 2 dicembre 2025
Centro Congressi “Beniamino Andreatta”
Arcavacata di Rende (CS)**





DFT investigation of hydroquinone decomposition on nickel

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Biomass has emerged as the only viable carbon source capable of replacing petroleum while reducing environmental pollution. Amid the various types, lignocellulose-rich biomass stands out as a promising candidate, primarily because it is a non-edible waste product and does not compete with the human food chain. Among the three biopolymers that compose it, namely cellulose, hemicellulose and lignin, the latter is the most thermally stable and unique in its potential to provide aromatic-based compounds. Hence, identifying the most efficient way to achieve a selective conversion of lignocellulosic biomass into value-added liquid fuels, known as bio-oils, constitutes an open field of research. Pyrolysis is one of the most extensively studied methods for transforming lignin into bio-oils; however, it often yields a broad and unpredictable distribution of products, complicating separation and raising processing costs. In this context, heterogeneous catalysis plays a key role in improving the efficiency and selectivity of biomass conversion. Additionally, quantum chemistry can provide crucial atomic-level insights into catalytic mechanisms, further supporting the rational design of effective catalysts.

In this study, Density Functional Theory in the SIESTA formulation was employed to investigate the pyrolysis of hydroquinone, a model compound for lignocellulosic biomass, on a Ni(111) surface represented by a 5x6 three-layer slab. The computational analysis maps out the energy barriers and reaction intermediates involved in the catalytic decomposition of hydroquinone into benzene and cyclopentene derivatives together with smaller molecules, such as ethylene, acetylene and CO (see Figure 1 below).

While the initial steps of pyrolysis involve the removal of oxygenated functional groups, the process proceeds at higher temperatures to include the cleavage of multiple carbon–carbon bonds, leading to the formation of small hydrocarbons and even the deposition of isolated carbon atoms on the catalyst surface. This latter phenomenon may result in surface carburization, which was evaluated as a plausible scenario based on the calculated energy barriers associated with the removal of elemental carbon. All the detailed DFT-derived energetics for the proposed decomposition pathways can be employed to perform a microkinetic analysis, for example by means of the Simplified Christiansen Method. This would enable an unbiased estimation of kinetic rate constants at specific temperatures and allow the identification of the most favourable reaction routes, ultimately determining the product distribution.

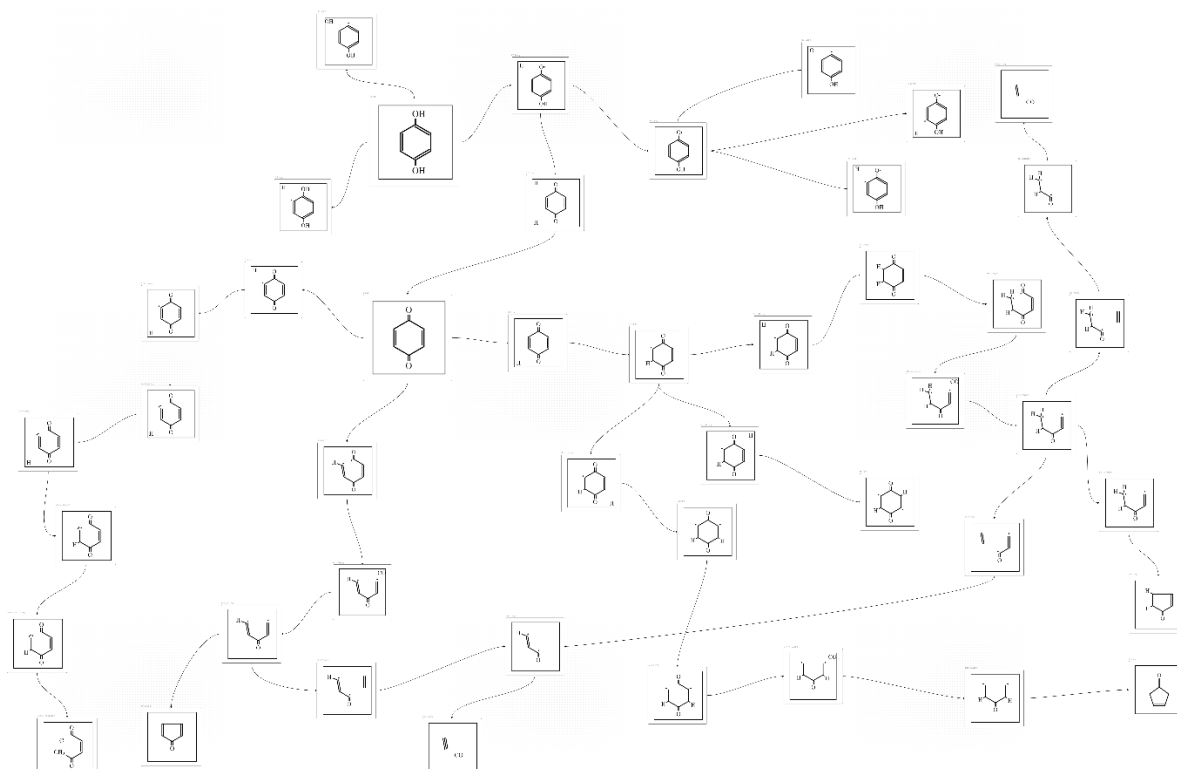


Figure 1: A schematic representation of the hydroquinone decomposition pathways investigated.

Acknowledgements: Authors acknowledge financial support under the National Recovery and Resilience Plan (PNRR), Mission 4, Component 2, Investment 1.1, Call for tender no. 104 published on 2.2.2022 by the Italian Ministry of University and Research (PRIN2022), 2022EX89KF, funded by the European Union Next-Generation EU-Project Title “An integrated environmental sustainable approach for the valorization of wet AGROindustrial wastes to bioMETHane” (AGROMET)–CUPB53D23005960006.