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A theoretical study of the influence of soot on the oxidation of PAHs by OH

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Understanding the aviation's impact on atmospheric chemistry, radiative forcing, and climate change, is a challenging task of great importance. In spite of the efforts undertaken to date by the scientific community, there is a lack of knowledge about the structure, the morphology, the composition, and the physico-chemical properties of aircraft engine soot that are released in the atmosphere.

We present here a modelling study of soot particles and of their interaction with Polycyclic Aromatic Hydrocarbons (PAHs). This work aim at better understanding, at the molecular level, the chemical reactivity at the surface of soot which is suspected to modify the atmospheric chemistry by providing surfaces for heterogeneous reactions. More specially, we focus on the oxidation process of PAHs by the OH radical. Because ab initio calculations on such large systems are not realistic, we have developped, in the present work, mixed classical/semi-empirical calculations to characterize this oxidation process on small graphite clusters modeling soot surfaces.