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Dissociative low-energy Electron Attachment (DEA) to deuterated methane CD_4 in adsorbed phase

Low energy electrons (LEE, typically 0-15 eV) are omnipresent in nature and play an important role in various natural phenomena as well as in many industrial processes. They allow in particular to break molecules via a dissociative attachment. Schematically, EBEs can attach to an AB molecule and form a transient anion (TA, AB^{-*}). This one can then relax via the dissociative electronic attachment process AED, forming a stable anion B^- and a neutral fragment A. The efficiency of the EBE attachment, the lifetime of the TAs strongly depend on the environment of the target molecules and in particular on the surface where the dissociative attachment is performed. In this context, the desorption of B^- is also strongly influenced by the surface.

In my PhD work, we have experimentally and numerically studied the dissociative electronic attachment of the deuterated methane molecule deposited on a platinum surface. CD_4 films of different thickness were deposited on Pt(111). The analysis of the desorption of D^-, CD^-, CD_2^- and CD_3^- anions was performed by mass spectrometry (Pr. Léon SANCHE Sherbrooke, Canada). This analysis revealed a desorption order $D^- >> CD_2^- > CD^- > CD_3^-$. We have also calculated the adsorption energies of the fragments that can be derived from the fragmentation of CD_4 on such surface and the excited states of CD_4 and CD_4^- in the gas phase that give rise to these fragments. These calculations provide insight into the role of the surface on the desorption of these anions. The calculations of the adsorption energies allow us to understand the order of desorption of the anions observed experimentally with the exception of CD_3^-. The calculated excited states give us information on the detection efficiency of the measured anions. Finally, the study of CD_4 films using a xenon spacer showed a higher DEA efficiency than on the clean surface.