Computational design of novel materials for CO_2 capture

Several high-profile inter-governmental programs (Horizon2020, IPCC, COP21, etc) have been established to fight climate change and the implementation of carbon capture has been proposed as a means of enabling the continued use of fossil fuels in the near term, while renewable energy resources gradually replace our existing infrastructure.

Available carbon capture technologies, however, are too expensive and would increase the cost of electricity significantly, making their implementation on large scale impractical. We seek a postdoc candidate to work on the development of an original way of efficiently capturing and releasing CO_2 from post-combustion processes. It consists in computationally designing functionalized metal-organic frameworks (MOFs), starting from available experimentally synthesized structures, which can use light irradiation as a way of tuning the affinity of the material for CO_2. In this way, CO_2 uptake can be dramatically reduced upon light treatment allowing for a substantial reduced energy consumption. The work will involve the use of several computational methods (from DFT to quantum chemistry to the use of excited state methods, and, depending on the candidate, also classical molecular dynamics). The specific focus of the project regarding how the methods will be combined together will be established together with the candidate prior to the project submission.

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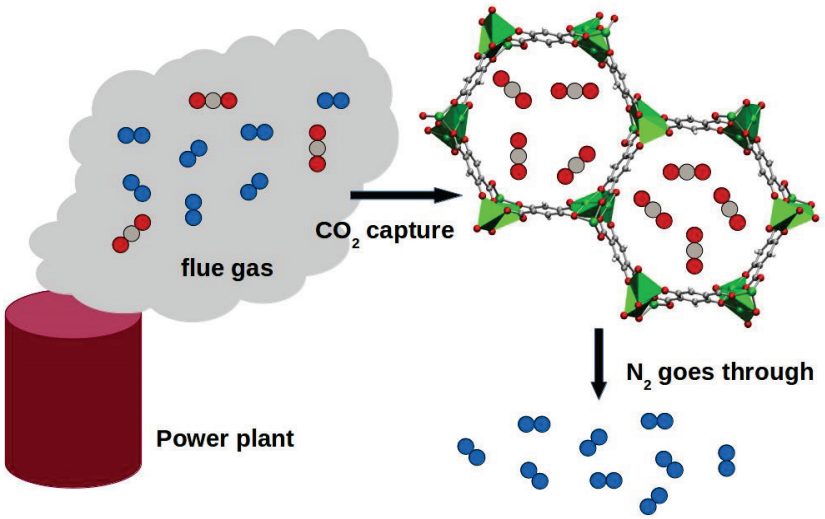
Web page



Sketch of a postcombustion capture process that uses MOFs. The flue gas contains 15 % of CO_2 and 75 % of N_2. Due to the low pressure of the flue gas (1 atm), the MOF should exhibit an extremely high affinity for CO_2 which can be modified with light treatment.