The discovery of graphene and its unique electronic properties has created interest in the potential of two-dimensional carbon-based materials for photo- and electrocatalytic applications. They offer nearly limitless possibilities for functionalization, for example by the amount of incorporated non-carbon atoms (in particular hydrogen, nitrogen, and oxygen) or the porosity, through which one may control activity and selectivity. However, this vast design space also necessitates a deep understanding of structure-property relationships, which can be obtained with the help of computational models. Density functional theory (DFT) is the method of choice due to a good compromise between computational time and accuracy. In this project, we plan to investigate different classes of two-dimensional carbon-based materials. We use water splitting as a model reaction and systematically investigate properties that are key parameters in their photo- and electrocatalytic performance, such as band gaps and free energies of the relevant reaction steps. This will allow us to identify reactivity descriptors that can be used to guide the design of improved catalysts.