Title: **A study of interatomic potentials in Au-MgO catalysts**

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Date: June 2019

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Interatomic potentials are mathematical functions key to understand and explain the behaviour of metallic clusters that form heterogeneous catalysts. Even though they are very important, there is not a reliable and standardized method to work with them for every case. In this project, we will work based on some semiempirical potentials to optimize them and try to expand their use for Au-MgO clusters of every size. To do it, we will explore how can coordination be determined and what is needed to explain the coordination between metal atoms in the cluster and between the atoms in the cluster and the surface.

We will try to systematise a way for any researcher interested in a mathematical function to explain the behaviour of the coordination in any cluster adsorbed on a surface. Our approaches will prove to be quite successful for the structures we studied, but that may not be the case for larger clusters. We will, however, try to give general rules that shall work no matter the size and shape of the cluster..