DFT based tight binding strategy for numerous atoms studies: properties of noble metal clusters and surfaces interacting with hydrogen atoms

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We first aim at developing new tools for the simulation of atomic and molecular clusters with the density functional based tight binding (DFTB) approach [1] that is used to generate the potential energy surface. After describing the DFTB method, it will be illustrated with a study of the energetic properties of noble metal cluster.

Additionally, preliminary results of the adsorption of H on the metal clusters will be presented focusing on the DFTB parameterization benchmarked on *ab initio* calculations.

The present work on clusters is a prerequisite towards a systematic investigation of the adsorption and reaction of hydrogen atoms on the (100) and (111) surfaces of silver and gold. For example preliminary DFT calculations [2] evidenced direct, non-activated H insertion paths into the bulk through the bridge and hollow sites of Ag(100). From this study it can be speculated that Ag(100) should be the ultimate system among pure transition metals to efficiently store atomic hydrogen. Thermal desorption spectroscopic measurements have indeed revealed a subsurface H population that can exceed that of the surface adsorbates depending on pre-exposure of H [3]. One puzzling and huge isotopic effect found is that surface reconstruction occurs with H but not with D.

The perspective is to use the DFTB approach in order to consider the interaction of more than just a few H atoms. To this aim classical molecular dynamics could be used in order to model the atomic hydrogen storage and the surface reconstruction, which could be validated upon comparison with quantum dynamical calculation on a smaller system.

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