Theoretical investigations of Ag/SiO_2 interface

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$Ag(111)/SiO_2$ system is of a great interest in optics, synthesis of new heterostructures, etc. In our work this interface was investigated by means of Density Functional Theory. All calculations were done using Quantum Espresso [1] package with plane-wave basis set and ultrasoft pseudopotentials for the treatment of the core electrons.

Different structures of $Ag(111)/SiO_2$ interface were considered and the size of lattices was chosen to reduce the strain at the interface. The influence of SiO_2 structure on the adhesion properties was investigated.

[1] P. Giannozzi et al., http://www.quantum-espresso.org.