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The structure, stability, and magnetic properties of Au(111)/NiO(111) interface: density functional theory study[1]

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We studied the electronic structure of Au(111)/NiO(111) interface in accordance with the two models of NiO(111) surface. The work of adhesion, the spin magnetic moment, the stability and the electronic properties of the Au(111)/NiO(111) interface were calculated by density functional theory (DFT). The calculated results of Au(111)/NiO(111) interface were then compared with non-polar Au(100)/NiO(100) interface. At the same time, the total density of states (DOS) of Au(111)/NiO(111) interface corresponding to the two models were also calculated. The calculations reveal that the Ni-terminated and the oxidized interfaces have antiferromagnetic properties, while the O-terminated interface exhibits ferromagnetic properties.

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