Monovalent adatom-induced $\sqrt{21}\times\sqrt{21}$ superstructures on the Ag/Si(111)-$\sqrt{3}\times\sqrt{3}$ surface : A first-principles study

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During the last decades the Ag/Si(111)-$\sqrt{3}\times\sqrt{3}$ surface has been intensively studied as a prototypical metal/semiconductor interface. A special property of the surface is that the submonolayer deposition of monovalent atoms (alkali- and noble-metals) induces a $\sqrt{21}\times\sqrt{21}$ reconstruction with drastically enhanced surface conductivity. It has been reported that the $\sqrt{21}\times\sqrt{21}$ phases induced by Ag, Au, Cu, and Na adatom show very similar band structures and scanning-tunneling microscope (STM) images, suggesting that the atomic structures of alkali- and noble-metal induced surface structures are basically the same. So far several structural models involving three,[1] four,[2] and five[3] adatoms per $\sqrt{21}\times\sqrt{21}$ unit cell have been proposed. However none of these models can explain the experimental observations of the $\sqrt{21}\times\sqrt{21}$ phase, and accordingly, a new structural model should be required.

In the present study, we suggest a new structural model possessing three adatoms per unit cell from density-functional calculations. In contrast to the previous models where all the adatoms sit above the Ag- or Si-trimers, extra adatoms in our structural model are adsorbed on the planar surface sites, resulting in the almost flat surface. The detailed atomic and electronic structure of the $\sqrt{21}\times\sqrt{21}$ phase as well as comparison with experimental results will be presented.

References

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