

## **512f The Effects of Contact Structures on the Electron Transport Characteristics of Au-Si Interfaces**

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Abstract An ab initio approach, which combines the Green's function technique for electron transport and density functional theory, is used to study the effects of the contact structures on the electron transport characteristics of Au-Si interfaces. The interface Hamiltonian is constructed from the Kohn-Sham Hamiltonian of the extended clusters and the density of states of the contacts. From the Green's function matrix, the density of states, the electron transport function and the current-voltage characteristics of the Au-Si interface are calculated. The electron transport function is very small when the energy of injected electron is below Fermi level. As the Si terminal is positively biased, electrons are more likely to tunnel through the Au-Si interface. On the other hand, as the Au terminal is positively biased, electrons are refrained from tunneling through the Au-Si interface. The number and geometry of the contact atoms has a large effect on the electron tunneling function.

Keywords electron transport, nanoelectronics, molecular electronics, Green's function, and density functional theory