

## Press Release

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### **Tuning surface d bands with bimetallic electrodes to facilitate electron transport across molecular junctions**

In many years, the Ministry of Science and Technology has been encouraging the scientific research. This research plan is under the long-term support of the Ministry of Science and Technology, Prof. Chun-hsien Chen and Prof. I-Wen Peter Chen have been created to turn surface d bands with bimetallic electrodes to facilitate electron transport across molecular junctions. This outstanding fundamental research result was published in the top journal 《 Nature Materials 》 in 2021.

Understanding chemical bonding and conductivity at the electrode–molecule interface is key for the operation of single-molecule junctions. Here we apply the d-band theory that describes interfacial interactions between adsorbates and transition metal surfaces to study electron transport across these devices. We realized bimetallic Au electrodes modified with a monoatomic Ag adlayer to connect  $\alpha,\omega$ -alkanoic acids ( $\text{HO}_2\text{C}(\text{CH}_2)_n\text{CO}_2\text{H}$ ). The force required to break the molecule–electrode binding and the contact conductance  $G_{n=0}$  are 1.1 nN and 0.29  $G_0$  (the conductance quantum,  $1 G_0 = 2e^2/h \approx 77.5 \mu\text{S}$ ), which makes these junctions, respectively, 1.3–1.8 times stronger and 40–60-fold more conductive than junctions with bare Au or Ag electrodes. A similar performance was found for Au electrodes modified by Cu monolayers. By integrating the Newns–Anderson model with the Hammer–Nørskov d-band model, we explain how the surface d bands strengthen the adsorption and promote interfacial electron transport, which provides an alternative avenue for the optimization of molecular electronic devices.

Establishing a solid base of fundamental research is crucial for the future advance of the high-tech industry in Taiwan. The success of this research

project also represents a milestone for in the research of fundamental science in Taiwan and meets the objectives of the program.

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