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N-Heterocyclic Carbene-Treated Gold Surfaces in Pentacene Organic Field-Effect Transistors: Improved Stability and Contact at the Interface

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Abstract: N-Heterocyclic carbene (NHC) molecules, which reacted with the surface of Au electrodes, have been successfully applied in the pentacene transistors. With the application of NHCs, the charge carrier mobility of pentacene transistors increased by five times, while the contact resistance at the pentacene-Au interface reduced down to 85%. Even after annealing the NHC-Au electrodes at 200 °C for two hours before pentacene deposition, the charge carrier mobility of the pentacene transistors did not decrease. The distinguished performance renders the NHCs as excellent alternatives to thiols as metal modifiers for the application in organic field-effect transistors (OFETs).

Surface modification of metal electrodes, especially on gold due to its inertness towards oxidation and corrosion, can optimize the charge injection at the metal-organic interface, which is remarkably important for the fabrication of high performing organic field-effect transistors (OFETs).[1] Hitherto various modifiers have been applied on gold surfaces including physisorbed polymers,[1b] barium salts,[2] chemisorbed graphene oxide,[3] and self-assembled monolayers (SAMs) of thiols.[4] In particular, since the ground-breaking report of dithiol SAMs on gold substrates 30 years ago,[4d] thiols on Au have become the mostly used combination due to their easy preparation, tunable properties throughout the chemical modification and the molecular order they provide. However, thiol monolayers completely desorbed in a low temperature range between 100-150 °C and even degraded within 1-2 weeks at room temperature in air.[4b, 4c, 4e, 5] Though longer-chain thiols and multidentate sulfur-based adsorbents slightly improve the stability of thiol SAMs, new alternatives that could form stronger bonding with gold would be more promising to improve the stability.

N-Heterocyclic carbenes (NHCs) are carbenes typically flanked by one or two heteroatoms adjacent to the carbene carbon. These heteroatoms can greatly improve the stability of the carbene species which enables synthesis and isolation of free carbenes of this type on gram scale from inexpensive

precursors such as imidazolium salts.[6] Structural modification can be easily realized by varying the N-substituents or the backbone of the NHCs. NHCs exhibit a strong σ-donating and moderate π-accepting ability which renders them as privileged ligands which form very stable complexes with late transition metals like Au(I), indicating a promising new system for metal surface modification. To date, there are only five literature reports[7] about the NHC-assembly on planar gold surfaces, whereas several nanoparticle-NHC systems were reported since 2009.[8] Crudden *et al.* successfully addressed the superior stability of NHC-modified Au surfaces (as compared to thiols) even under various harsh conditions including submersion in boiling water or exposure to 1% H_2O_2 for 24 hours.[7a] Moreover, electronic studies demonstrate that the NHC-Au bond is highly conductive and stabilized by conjugation.[7b] Specially, its HOMO electron density is delocalized over the gold atom, the carbene carbon and even the nitrogen atoms. The strength of the NHC bonded to a gold surface has been measured to be around 20 Kcal stronger[7a, 7b, 9] than Au-S bonds (40-50 Kcal).[4c, 10] These results imply that NHCs could serve as potential alternatives to thiols for the application in metal surface modification.

Herein, we report the first modification of the metal-organic interfaces of OFETs with NHC molecules. Relative to pure Au electrodes, the optimized NHC-functionalized gold electrodes substantially lowered the Au-pentacene contact resistances up to 85% and enhanced the carrier mobility by a factor of five. Most importantly, the NHC-functionalized Au surface was stable up to 250 °C, a significantly higher temperature than thiol-functionalized Au surfaces are able to withstand.[4b, 4c, 4e]
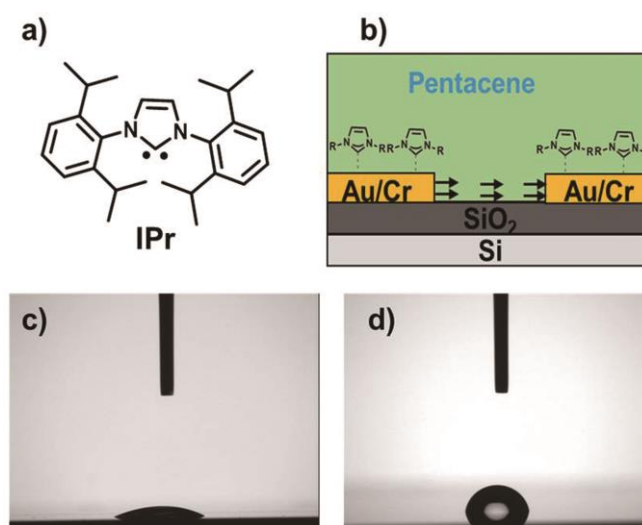

Figure 1. a) Chemical structure of IPr; b) Schematic diagram of a bottom-gate bottom-contact (BGBC) OFET with pentacene as the organic

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semiconductor; c) Contact angle of water on Au surface and d) contact angle of water on IPr-functionalized Au surface.

The chemical structure of NHC IPr is shown in Figure 1a. IPr was first synthesized according to a literature procedure (Scheme S1, S2).[11] It is then reacted with Au surfaces upon immersion of pre-patterned Au electrodes into corresponding NHC solutions in toluene at room temperature. The contact angle increased from around 40° to 85° after this reaction (Figure 1c, 1d). X-ray photoelectron spectroscopy (XPS) indicated both the nitrogen and carbon signal on the Au surface. The shift of the C-N bond detected corresponds to that of a carbene (Figure S1-S3). Upon thermal annealing in air, the IPr-Au bonds withstood high temperatures until 250 ^{o}C. At 250 ^{o}C, the contact angle of water on the IPr-Au surface decreased to nearly zero degrees (Figure S4). Pentacene was then deposited onto the NHC-Au electrodes by vacuum evaporation as shown in Figure 1b. The fabricated OFET devices had the same channel width of 1 mm and different channel lengths of 40 μm, 55 μm, 70 μm, 90 μm and 125 μm.

Three concentrations of IPr in toluene (1 mM, 5 mM and 10 mM) were investigated. For each concentration, we measured about fifty pentacene transistors and all the devices were measured under ambient conditions. The pentacene transistors with pure Au electrodes showed an average hole mobility of 0.03 $cm^2V^{-1}s^{-1}$ (Figure 2a&b, Table 1), which was comparable to the reported results under similar conditions.[12] Among the three concentrations, transistors treated with 5 mM IPr showed the highest hole mobility, whose average value was 0.15 $cm^2V^{-1}s^{-1}$ and was five times higher than transistors
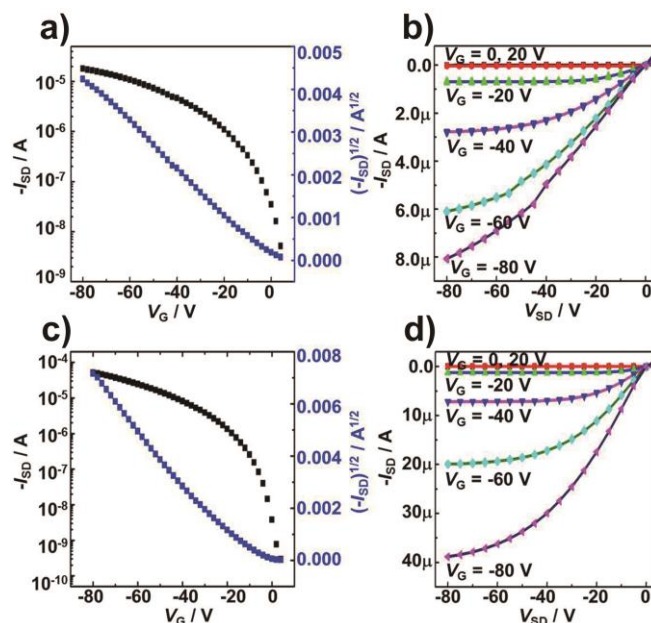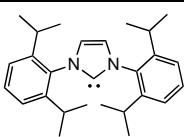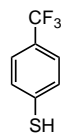

Figure 2. Typical transfer curve a) and output curve b) of pentacene transistor with bare Au electrodes; and typical transfer curve c) and output curve d) of pentacene transistor with 5 mM IPr-functionalized Au electrodes.

without IPr (Figure 2c&d). Modifications of Au electrodes using 1 mM and 5 mM solutions of IPr greatly improved the hole mobilites (μ) of the pentacene transistors, compared to pure Au electrodes, but hardly changed the threshold voltages (V_T) and current on/off ratios ($I_{ON/OFF}$) at all (Table 1). When the IPr

Table 1. Performance summary of pentacene transistors with bare, IPr and TFMBT-modified Au electrodes.

SAM	Concentration	μ/cm^{2}V^{-1}s^{-1}	V_T/V[a]	I$_{ON/OFF}$[a]	Resistance/MΩ[a]
Au	---	3.0E-2	−4.1	2.0E5	5.5
IPr	1 mM	8.6E-2	-6.2	2.6E5	2.0
	5 mM	**1.5E-1**	**-3.9**	**2.3E5**	**0.9**
	10 mM	2.0E-2	-5.2	8.2E3	8.3
	5 mM, Annealing[b]	**1.7E-1**	**-7.1**	**2.7E5**	---
TFMBT	5 mM	6.0E-2	-2.0	1.6E4	---
	5 mM, Annealing[b]	3.4E-2	-0.9	1.3E3	---
	10 mM	8.6E-2	-1.5	5.8E3	---
	10 mM, Annealing[b]	4.5E-2	-5.3	3.6E4	---

[a] Average value over fifty devices. [b] Au electrodes with SAM modifiers were annealed at 200 ^{o}C for 2 hours.

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concentration was increased to 10 mM, both the hole mobility and current on/off ratio dramatically decreased, but the threshold voltage still showed negligible variation. These results indicate that modification of Au electrodes with IPr had little effect on the V_T of pentacene transistors. More importantly, the hole mobility of the pentacene transistors did not decrease even after annealing the 5 mM IPr-Au electrodes at 200 ^{o}C for 2 hours before pentacene deposition. The pentacene transistors with annealed electrodes gave an average mobility of 0.17 cm^{2}V^{-1}s^{-1} over fifty devices, which was comparable to that of pentacene transistors with unannealed electrodes (Table 1).

The S-Au bonds formed through immersing pre-patterned Au electrodes into isopropanol solution of 4-(trifluoromethyl)benzenethiol (TFMBT) were also studied for comparison. Two concentrations were explored (5 mM and 10 mM). The average hole mobilities (0.06 cm^{2}V^{-1}s^{-1} and 0.086 cm^{2}V^{-1}s^{-1}) were measured in air separately for fifty pentacene transistors functionalized in solutions of 5 mM and 10 mM. Wherein 10 mM TFMBT gave a higher hole mobility, which is consistent with previous results in the literature (Table 1).[13] Compared to pure Au electrodes (0.03 cm^{2}V^{-1}s^{-1}), both concentrations of TFMBT could improve the hole mobilities of pentacene transistors. But in contrast to transistors functionalized with IPr (0.15 cm^{2}V^{-1}s^{-1} at 5 mM), the transistors modified with TFMBT exhibited much lower mobility under the optimized concentration. After heating the electrodes with TFMBT at 200 ^{o}C for 2 hours in air before pentacene deposition, the hole mobility of transistors with TFMBT at both concentrations dramatically decreased and nearly diminished to that of transistors with pure Au electrodes (Table 1). Compared with TFMBT, the use of IPr as an electrode modifier greatly increased the thermal stability of the pentacene devices. In short, N-heterocyclic carbenes turn out to be excellent substitutes as modifiers for Au electrodes in OFETs
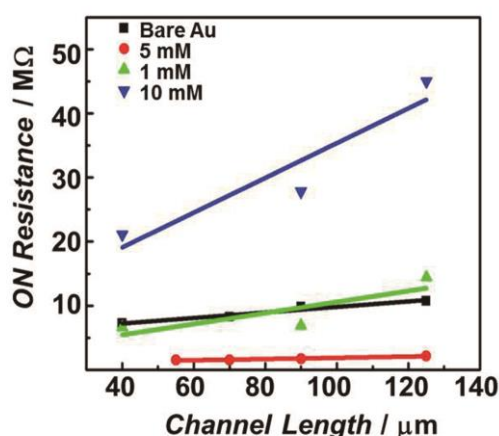

Figure 3. Plots of ON resistances versus various channel lengths in the pentacene transistors. Four lines separately represent the ON resistances of transistors with 1 mM (green), 5 mM (red), 10 mM (blue) and without (black) IPr.

In an OFET device, the contact resistance between semiconductor and the gold electrodes changes once the modifier assembles on the gold surface. Consequently, in addition to evaluating the μ, V_T and $I_{ON/OFF}$, another useful

means of comparison is the contact resistance of the bare vs. IPr-modified pentacene transistors. If we neglect the space charge limited current effect, the OFET ON resistance (R_{on}) in the linear region, where the source-drain voltage is much lower than the gate voltage, can be expressed in the following equation:[12b, 14]

$$R_{on} = R_{ch}L + R_{S/D} \qquad (3)$$

R_{ch} represents the channel resistance of unit length, L indicates the channel length and $R_{S/D}$ denotes the contact resistance. The contact resistance can be extracted by first measuring the ON resistance from the linear region of the OFET output curve (Figure 2b&d) and then by plotting the ON resistance as a function of channel lengths (Figure 3). Pentacene transistors with five channel lengths (40 μm, 55 μm, 70 μm, 90 μm and 125 μm) but the same channel width (1 mm) were measured. According to equation 3, we could obtain the contact resistances by extrapolating the linear relationship of R_{on} versus L to L=0 as shown in Figure 3. All the ON resistances were measured at low source-drain voltage of -5 V and high gate voltage of -80 V. The calculated contact resistance of pure Au electrodes was around 5.5 MΩ, which was consistent with the results in the previous reports.[12b, 15] This verified that equation 3 could be used to express the resistance of pentacene transistors. In the same way, contact resistances with three IPr concentrations were calculated as shown in Table 1. At a concentration of 1 mM, the IPr-assembling on the Au surface reduced the contact resistance at the Au/pentacene interface to 2.0 MΩ. After modification of the Au surface using the higher concentration of 5 mM IPr, the contact resistance further decreased to 0.9 MΩ. Compared to pure Au electrodes, Au-electrodes exposed to a 5 mM solution of IPr in toluene showed a decreased contact resistance at the Au-pentacene interface up to 85%. When the concentration of IPr increased to 10 mM, however, the contact resistance rose to 8.3 MΩ. Atomic Force Microscopy (AFM) was then used to characterize the morphological characteristics of the pentacene film at the interface. We found the pentacene film at the 5 mM IPr-Au/pentacene interface had the clearly largest grain size (Figure 4a&4b, Figure S5a&S5b), which is consistent with the highest hole mobility and the lowest contact resistance.[16] The above results demonstrate that 5 mM was the best concentration for the reaction of IPr with the Au surface. The optimal concentration is very important to obtain the best OFET performance. Changing the concentration of the IPr solution could tune the structure and macroscopic properties of the IPr-assembling on the Au surface.[17]
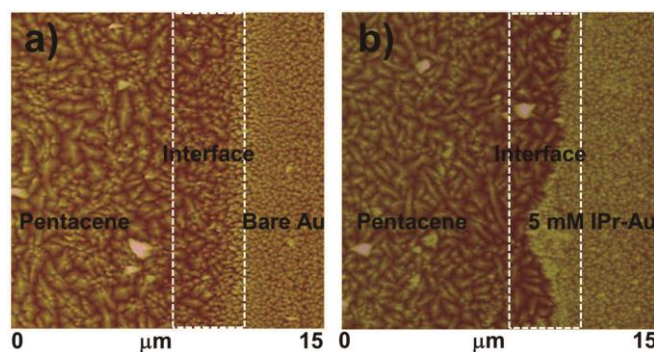

Figure 4. AFM characterization of (a) pure Au/pentacene interface; and (b) 5 mM IPr-functionalized Au/pentacene interface.

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Table 2. The charge carrier mobilites (μ) and calculated work functions for gold surfaces modified with three NHCs.[7e]

NHCs	Chemical Structure	Work Function /eV	μ /cm^{2}V^{-1}s^{-1}
Au	---	5.17	3.0E-2
IPr		4.13	1.5E-1
iPr$_2$bimy		3.90	7.8E-2
IiPr		3.84	4.5E-2
Pentacene	---	5.0	---

Furthermore, we investigated the characteristics of pentacene transistors with Au electrodes modified by the NHCs iPr$_2$bipy and IiPr (Table 2). Compared to IPr, these two NHCs showed larger grain size of pentacene films at the interfaces (Figure S5d& S5e) but much lower mobilities. Hence the morphological characteristics at the interface could not explain the OFET performance of pentacene transistors. DFT calculations indicate that NHCs can reduce the work function of Au surfaces while IPr leads to slightly smaller reduction of the work function compared to iPr$_2$bimy and IiPr.[7e] We attribute this effect to the additional coordination of the aromatic substituents to the Au surface. Among the three NHCs tested, the work function of the Au surface modified with IPr shows the smallest difference to the HOMO of pentacene (-5.0 eV).[15, 18] Therefore, compared to pure Au electrodes, the charge injection was greatly enhanced, indicated by the maximal current increase from 18 μA to 51 μA (Figure 2a&2c). Though the work function of pure gold mostly matches the HOMO of pentacene, it seems that the high charge trap density induced by the small grain size at the interface (Figure 4a) has largely deteriorated the OFET performance of pentacene transistors. Therefore, proper structure adjustments of the NHCs are important for OFET performance.

In conclusion, surface modifications of Au electrodes with NHCs have been successfully applied in pentacene OFET transistors. IPr displayed the best OFET performance among the three investigated NHCs. And 5 mM IPr in toluene was the best concentration for reaction of IPr with pre-patterned Au electrodes. Annealing experiments at 200 ^{o}C in air demonstrated that IPr-Au bonds were much stronger than the S-Au bonds. By using IPr as the electrode modifier, the pentacene transistors showed highly increased hole mobility from 0.03 cm^{2}V^{-1}s^{-1} to 0.15 cm^{2}V^{-1}s^{-1}, which was higher than that of pentacene

transistors modified with TFMBT thiol (0.086 cm^{2}V^{-1}s^{-1}). The increased OFET performance should be attributed to the decreased contact resistance induced by: a) the increased grain size at the IPr-Au/pentacene interface; and b) the enhanced charge injection as a result of the IPr-assembling on the Au surface. In summary, we have demonstrated that IPr is an exceptionally valuable alternative to thiols as a modifier on the Au surface in the application of OFET devices.

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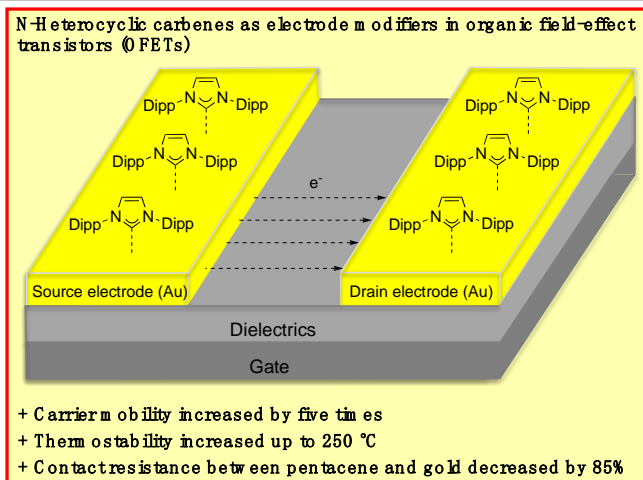
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N-Heterocyclic carbene (NHC) molecules have been successfully applied to modify the surfaces of Au electrodes in organic field-effect transistors (OFETs) in this work. The greatly improved transistor-performance and excellent thermal stability in air indicate that the NHCs would be excellent alternatives to thiols as metal modifiers for application in OFETs.

N-Heterocyclic carbenes as electrode modifiers in organic field-effect transistors (OFETs)

+ Carrier mobility increased by five times
+ Thermo stability increased up to 250 ℃
+ Contact resistance between pentacene and gold decreased by 85%

Aifeng Lv, Matthias Freitag, Kathryn M. Chepiga, Andreas H. Schäfer, Frank Glorius* and Lifeng Chi*

N-Heterocyclic Carbene-Treated Gold Surfaces in Pentacene Organic Field-Effect Transistors: Improved Stability and Contact at the Interface