Supporting Information for “Contact electrification of organic liquid - metal interface induced by energy level shift”

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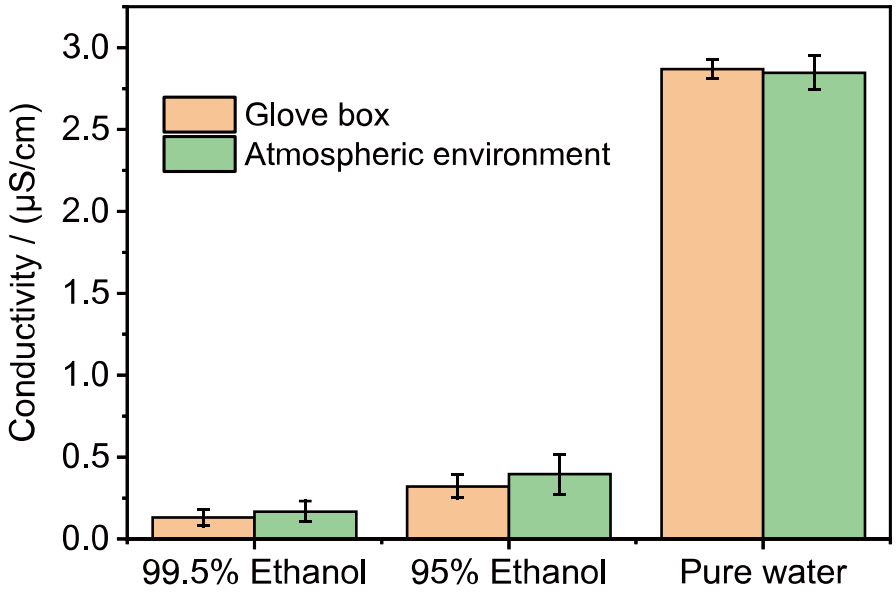

Figure. S1 The conductivity of 99.5% Ethanol, 95% Ethanol and pure water measured in the glove box and atmospheric environment, respectively.

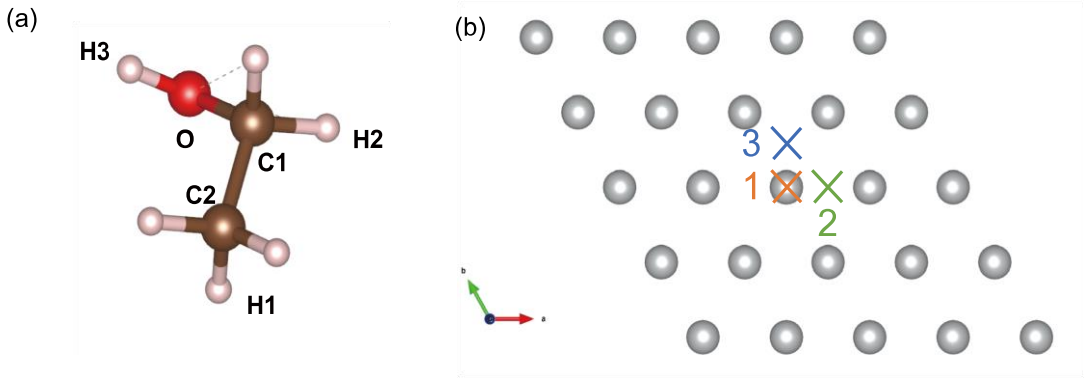

Figure. S2 Different adsorbed atom of ethanol molecule (H1, H2, H3, O, C1, C2) and the possible adsorption site on Ag atoms (1: top site, 2: bridge site, 3: hollow site).

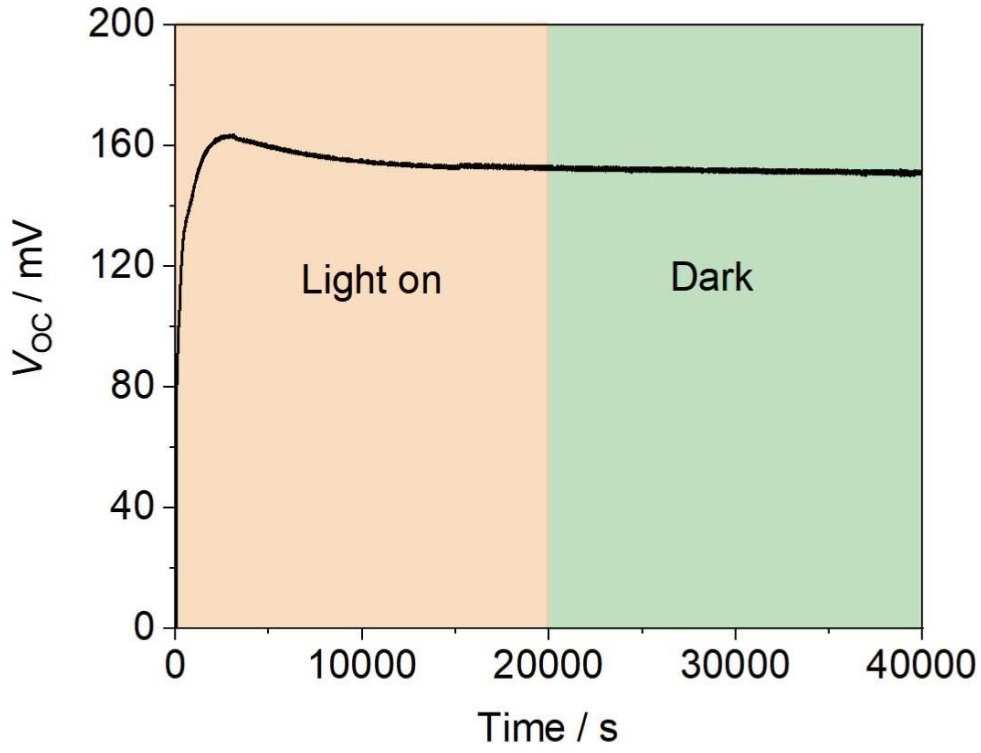

Figure. S3 Measured V_{OC} when Cu-Ag-ethanol system was covered by blackout fabric.

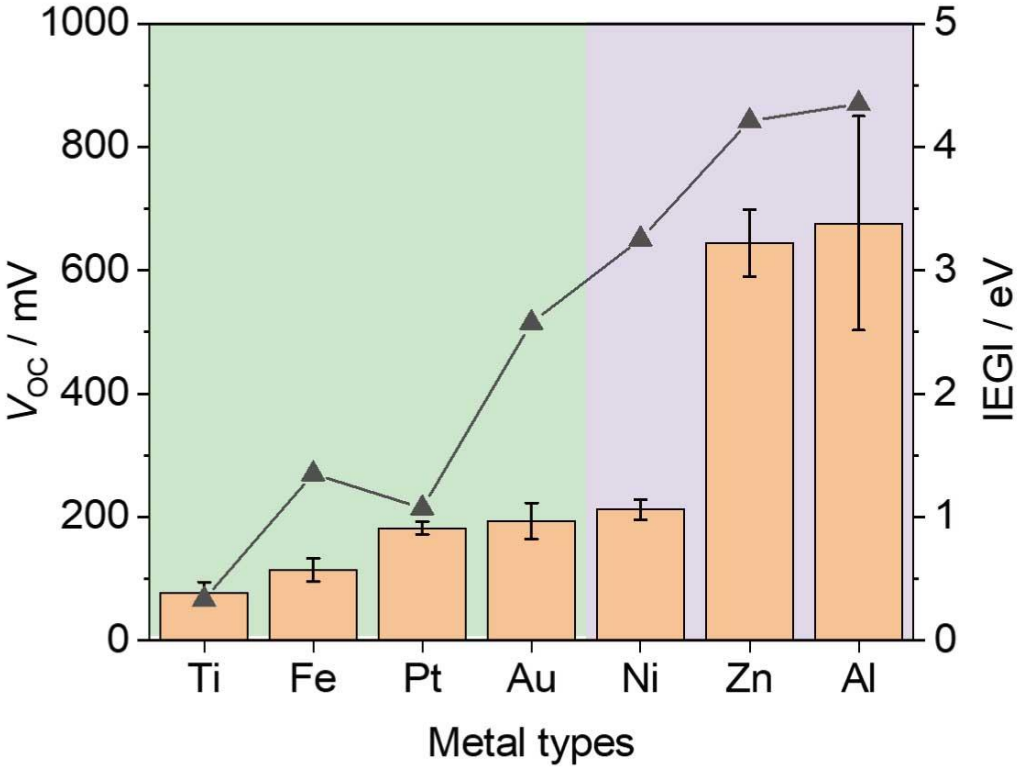

Figure. S4 Measured V_{OC} for various metal substrates, along with the barrier differences relative to the silver electrode in an ethanol environment.

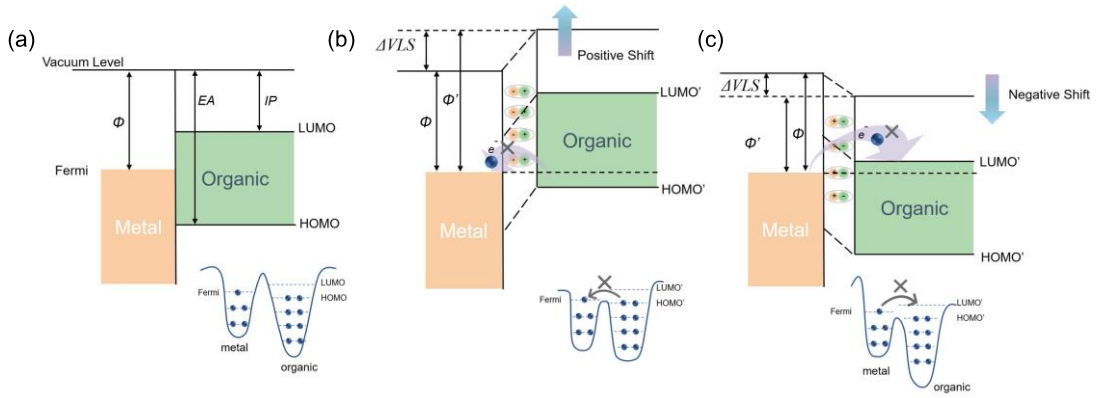

Figure. S5 (a) Initial energy level alignment at the metal-organic molecule interface prior to contact. (b) Positive vacuum energy level shift after contact, where the HOMO level of the organic molecule insufficient to rise above the Fermi level of the metal and lead to electron transfer from the organic molecule to the metal. (c) Negative vacuum energy level shift after contact, where the LUMO level of the organic molecule insufficient to fall below the Fermi level of the metal and cause electron transfer from the metal to the organic molecule.

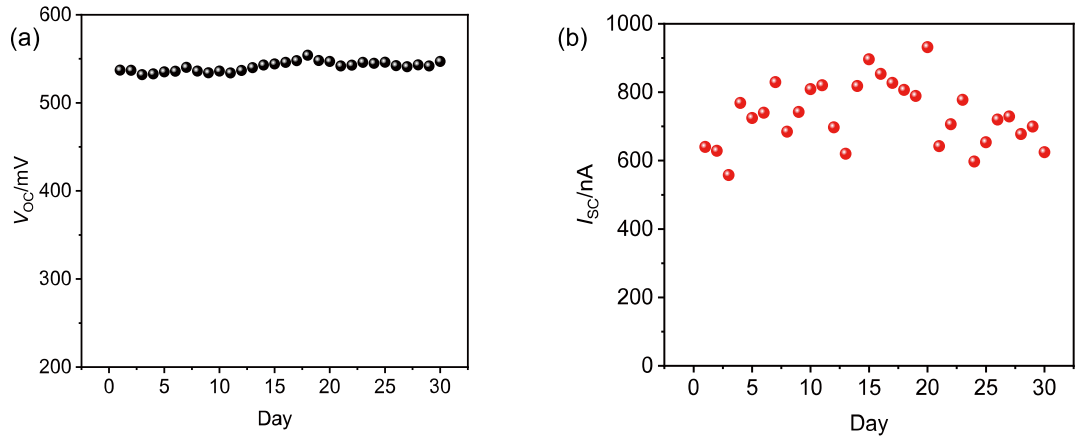

Figure. S6 (a) Cycling measurement of V_{OC} and I_{SC} during 30 days.

Table S1 The adsorption energy and electron transfer of different configuration

Adsorption configuration	Adsorption energy (E_{ads}) / eV	Electron transfer / e
Ag_C1_1	-0.1135	-0.0379
Ag_C1_2	-0.1006	-0.04341
Ag_C1_3	-0.1024	-0.03508
Ag_C2_1	-0.1501	-0.02486
Ag_C2_2	-0.1332	-0.02798
Ag_C2_3	-0.1319	-0.02802
Ag_O_1	-0.1007	-0.01902
Ag_O_2	-0.0822	-0.02412
Ag_O_3	-0.0765	-0.02541
Ag_H1_1	-0.0284	-0.03679
Ag_H1_2	-0.0295	-0.03702
Ag_H1_3	-0.0289	-0.03795
Ag_H2_1	-0.0471	-0.03175
Ag_H2_2	-0.0448	-0.03391
Ag_H2_3	-0.0445	-0.03393
Ag_H3_1	-0.0648	-0.04483
Ag_H3_2	-0.0642	-0.04434
Ag_H3_3	-0.0644	-0.04493

Table S2 The adsorption information after optimization

Adsorption configuration	Adsorption energy (E_{ads}) / eV	Electron transfer / e
Cu_Ethanol	-0.1501	0.022933
Zn_Ethanol	0.1934	-0.0612
Ti_Ethanol	-0.4911	-0.06711
Pt_Ethanol	-0.3782	0.051062
Al_Ethanol	-0.4182	-0.04684
Au_Ethanol	-0.0855	0.051671
Fe_Ethanol	-0.4554	0.03771
Ni_Ethanol	-1.0775	0.020135
Cu_DMSO	-0.9213	-0.05569
Cu_N,N-dimethylformamide	-1.1081	0.08517
Cu_Acetone	-0.0485	0.051879
Cu_Triethylamine	-2.9387	0.045685
Cu_Cyclohexane	-0.2525	-0.05886
Cu_Methanol	-1.5941	-0.04132
Ag_DMSO	-0.5455	0.039951
Ag_N,N-dimethylformamide	-0.7596	0.06886
Ag_Acetone	-0.393	0.041228
Ag_Triethylamine	-2.4444	0.053921
Ag_Cyclohexane	-0.5469	-0.02605
Ag_Methanol	-1.5941	-0.02839