Surface-Enhanced Raman Spectroscopic Study of 1,4-Phenylene Diisocyanide Adsorbed on Gold and Platinum-Group Transition Metal Electrodes

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Supporting information

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Supporting information 1

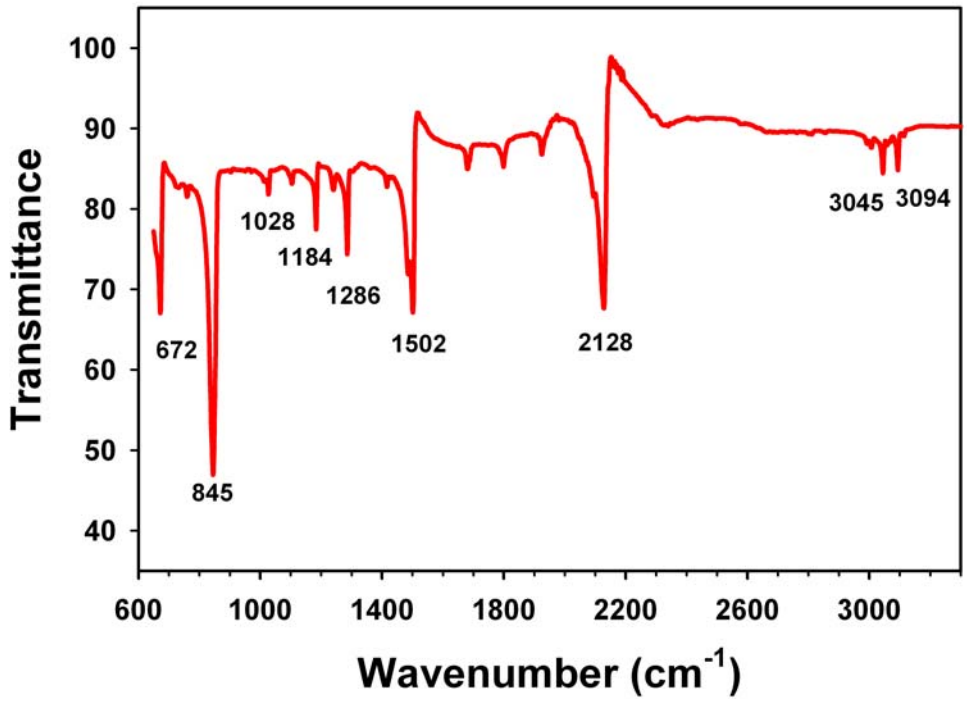

Figure S1. Transmittance IR spectrum of PDI powder. The band assignment is shown in Table 1.

Supporting information 2

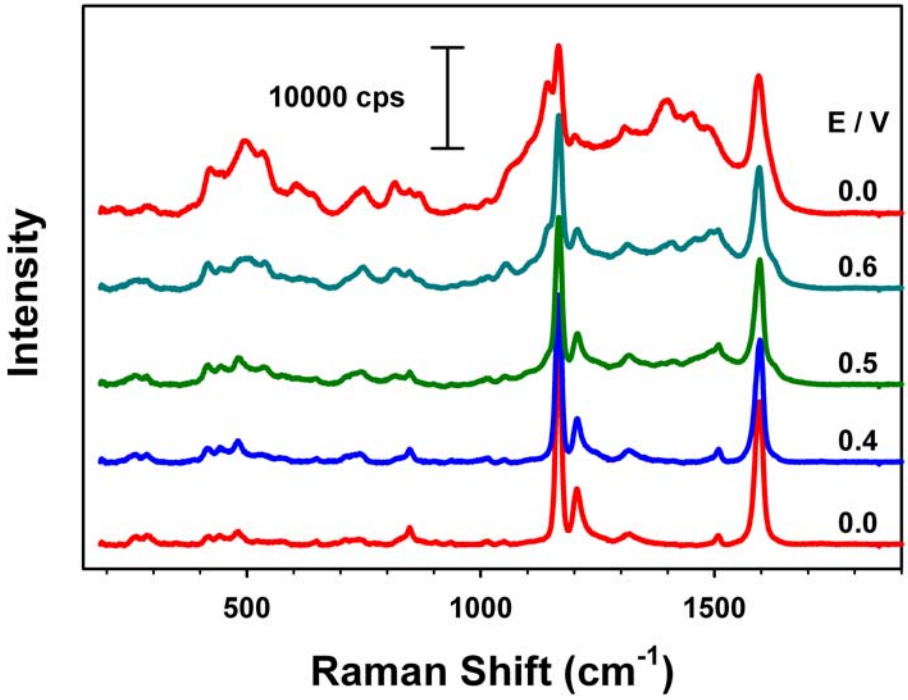

Figure S2. Potential-dependent SER spectra of PDI on Au in 0.1 M $NaClO_4$, demonstrating the effect of potential excursion to more positive than +0.4 V. The potential was stepped from 0.0 V first toward positive values up to +0.8 V then returned to 0 V in 0.1 or 0.2 V increment/decrement. Only selective spectra demonstrating spectral changes are shown. The top spectrum was recorded at 0.0 V after the potential was returned from +0.8 V. Spectrum acquisition time is 2 seconds.

Supporting information 3

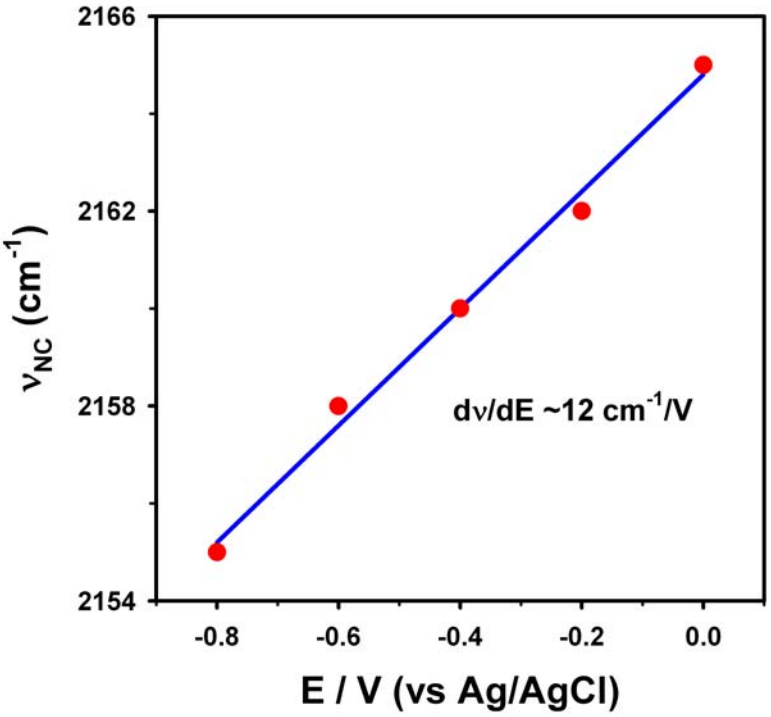

Figure S3. Peak frequency of N-C stretch for PDI adsorbed on Rh plotted as a function of applied potential. The data points are taken from the spectra in Figure 5B (see text).

Supporting information 4

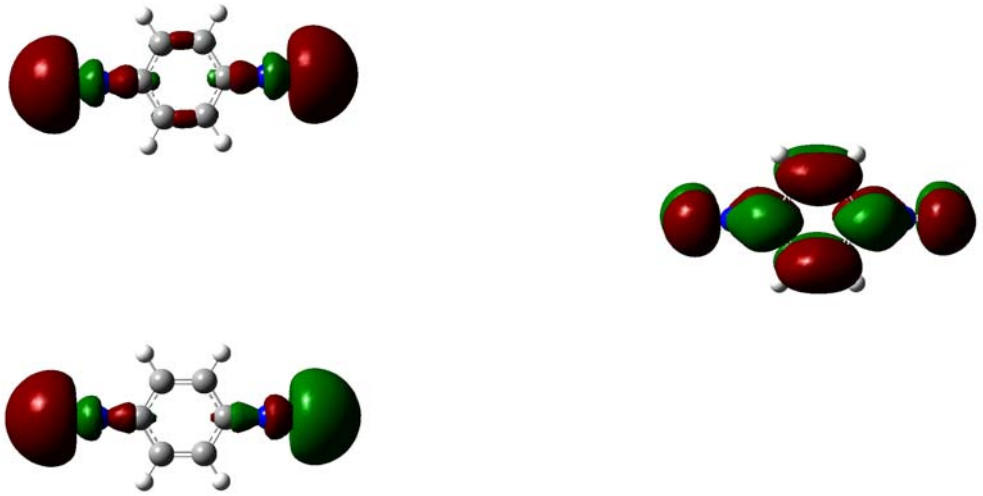

Figure S4. Molecular orbitals involved in PDI-metal bonding: (A) degenerate occupied orbitals for σ-donation; (B) π-back donation orbital. These orbitals are results from the DFT calculations (see text for details).