Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for Quantum Interference Effects in Biphenyl Dithiol for Gas Detection

Jariyanee Prasongkit*,† and Alexandre R. Rocha¶

†*Division of Physics, Faculty of Science, Nakhon Phanom University, Nakhon Phanom 48000, Thailand*

‡*Nanotec-KKU Center of Excellence on Advanced Nanomaterials for Energy Production and Storage, Khon Kaen 40002, Thailand*

¶*Instituto de Física Teórica, Universidade Estadual Paulista (UNESP), São Paulo, SP, Brazil*

E-mail: jariyanee.prasongkit@npu.ac.th

1 Initial Configurations

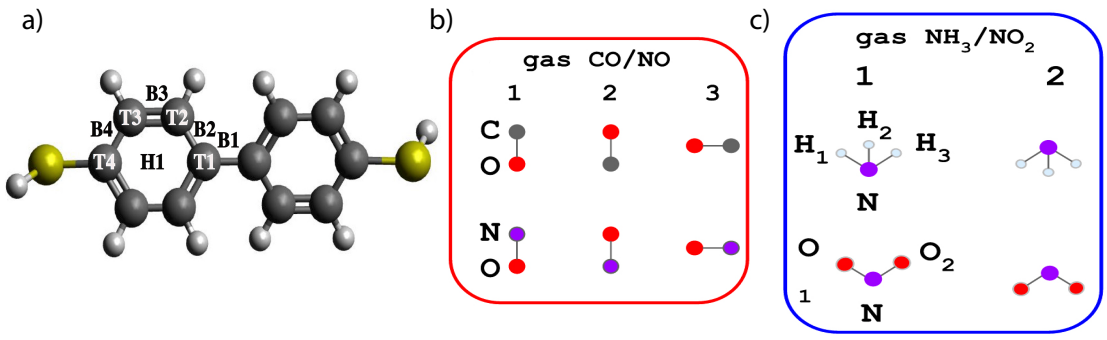

Figure S1: (a) Schematic structure and initial configurations of the biphenyl molecule (b) Different molecular orientations were examined for (b) CO and NO (diatomic gas molecules) with three possible orientations and (c) NH_3 and NO_2 (tri- and tetra-atomic gas molecules) with two initial orientations.

Figure S1-(a) shows initial configurations of gas adsorption on biphenyl molecule. Gas molecules were placed on possible adsorption sites of the biphenyl ring; position at the top of the C atom (T1-T4), position above the center of phenyl ring (H1), position above the bond (B1-B4). Owing to its molecular symmetry, each adsorption site of the first and the second phenyl rings showed no significant difference in the binding energy. Note that the starting configuration was not the final one.

For diatomic gases (CO and NO), we investigated three possible orientations. Their molecular axis was oriented parallel and with respect to the plane of biphenyl molecule. For tri- and tetra- atomic gases (NH_3 and NO_2), two orientations were tested, i.e., one with the N atom pointing to the surface and the other with the N atom pointing away from the surface. These can be seen in Figure S1-(b,c).

2 Stable configurations

The torsion angles ϕ of BPDT isolated molecule and BDPT with gas adsorption are shown in Table S1. Comparing to previous theoretical results[38], the torsion angle of BPDT isolated molecule agree quite well. Due to gas adsorption, we found the torsion angles slightly change. The binding distances in TableS1 indicate that gas molecules prefer adsorption onto the ring-connecting C atom (T1).

Table S1: Calculated torsion angle (ϕ) and binding distance.

molecule	Torsion angle (ϕ)	D (Å)
BPDT	36.58, (36.4) [38]	
BPDT+NO	36.25	T1–N=2.52, T4–O=2.89
BPDT+NO_2	35.97	T1–N=2.50,T4–O=3.16
BPDT+NH_3	37.01	T1–H=3.11, T1–N=3.41
BPDT+CO	37.03	T1–C=3.02, T4–C=3.26

3 Molecular-level analysis

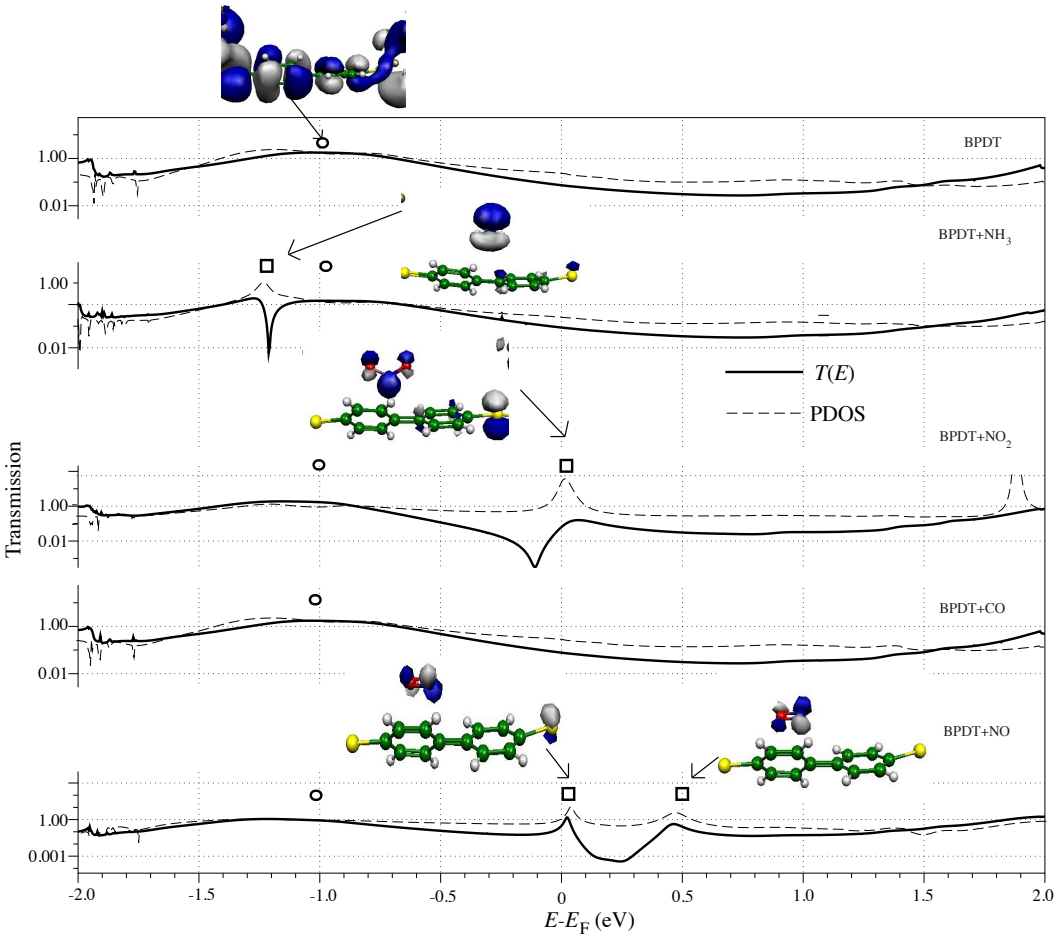

Figure S2: The transmission coefficients and PDOS of BPDT-Au junction with and without gas adsorption. The PDOS and transmission peaks associated with the HOMO of isolated nucleobases (circle) and molecular orbitals of gas molecules (square) are identified.

The HOMO level of BPDT gives rise to a broad transmission resonance peak below the Fermi energy ($E - E_F \sim -1$ eV). When NO and NO_2 is adsorbed on the BPDT, the sharp peaks in the PDOS observed around the Fermi energy arise from the localized states of gas molecules. The Fano resonance arises from the interference between the tail of the broadened HOMO of BPDT and the bound molecular states of NO and NO_2. For NH_3, we found the localized PDOS (bound state) of gas molecules superposes on the broad PDOS (continuum state) leading to an antiresonance in the transmission as seen in Figure S2.