Supporting information file

g-C_3N_4/CoN_4 Heterojunction as a Sensor for Detecting Volatile Organic Compounds: A Density Functional Study

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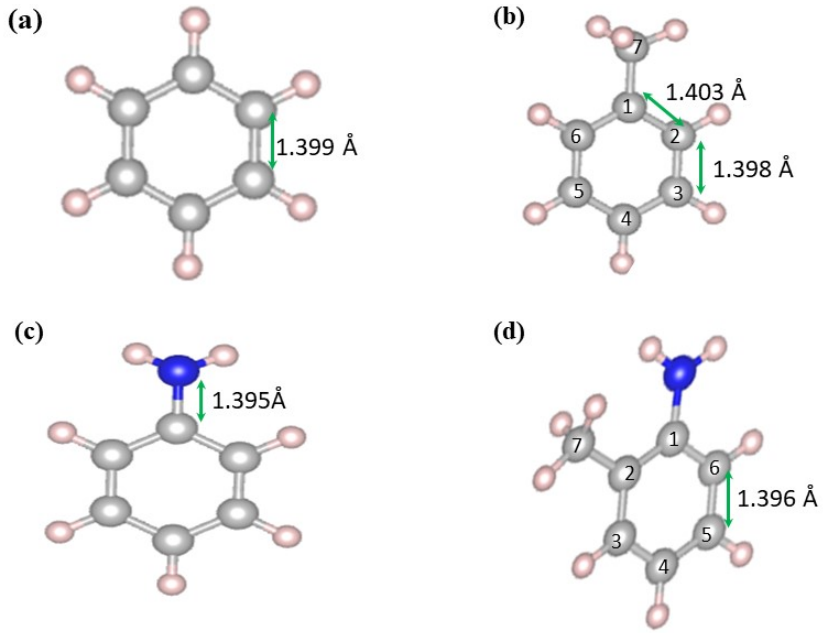

Figure S1: Optimised structures of biomarkers (a) Benzene, (b) Toluene (c) Aniline and (d) o-Toluidine

Table S1: Bond parameters of gas molecules

Parameter	Compound	Calculated value	Reference value
Bond length	Aniline (C-N)	1.395 Å	1.392 Å (1)
	Benzene (C-C)	1.399 Å	1.399 Å (2)
	Toluene (C1-C2)	1.403 Å	1.397 Å (4)
	Toluene (C2-C3)	1.398 Å	1.394 Å (4)
	O-toluidine (C-C)	1.404 Å	1.405 Å (5)
Bond angle	Aniline (N-C-C)	120^0	120^0 (1)
	Benzene (C-C-C)	$119^0 54'$	$119^0 28'$ (3)
	Toluene (C6-C1-C2)	119.40^0	119.40^0 (4)
	O-toluidine (N-C-C)	118.9^0	120.3^0 (5)

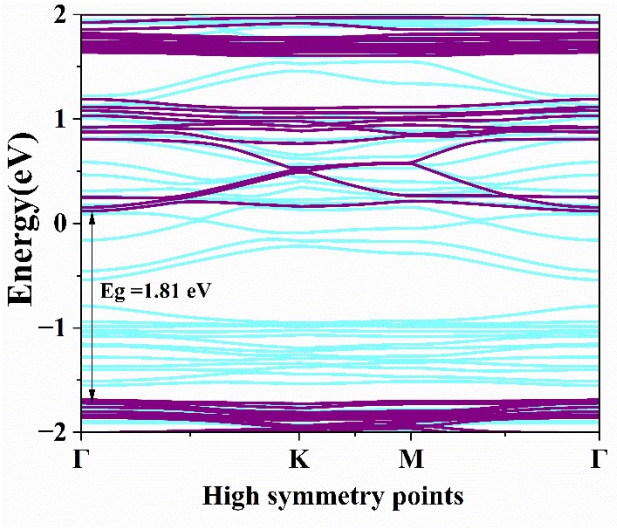

Figure S2: Band structure of g-C_3N_4/CoN_4 heterojunction

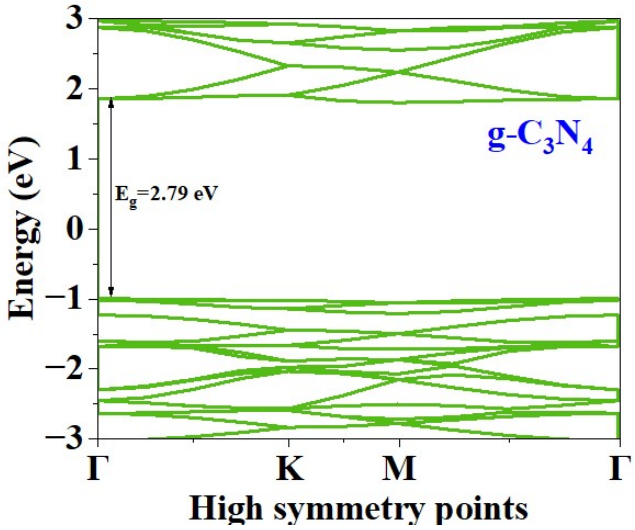

Figure S3: Band structure of g-C_3N_4 using HSE06 functional

References

(1) Vaschetto, M. E.; Retamal, B. A.; Monkman, A. P. Density Functional Studies of Aniline and Substituted Anilines. Journal of Moleclar Structure THEOCHEM 1999, 468 (3), 209–221,Mariana E. Vaschetto, Bernardo A. Retamal, Andrew P. Monkman.

(2) Tamagawa, K.; Iijima, T.; Kimura, M. Molecular Structure of Benzene. J. Mol. Struct. 1976, 30 (2), 243–253.

(3) Cox, E. G. Crystal Structure of Benzene. Rev. Mod. Phys. 1958, 30 (1), 159–162.

(4) Toluene: Structure, Dynamics, and Barrier to Methyl Group Rotation in Its Electronically Excited State. A route to IVR David R. Borst and David W. Pratt. J. Chem. Phys. 2000, 113, 3658.

(5) Bel'skii, V. K.; Chetkina, L. A.; Shuvaeva, V. A. STRUCTURE OF o-TOLUIDINE (CI4HI6N2). Repeated DETERMINATIONUDC, 548.737