Engineering Sensitivity: Sensors for Toxic Gases

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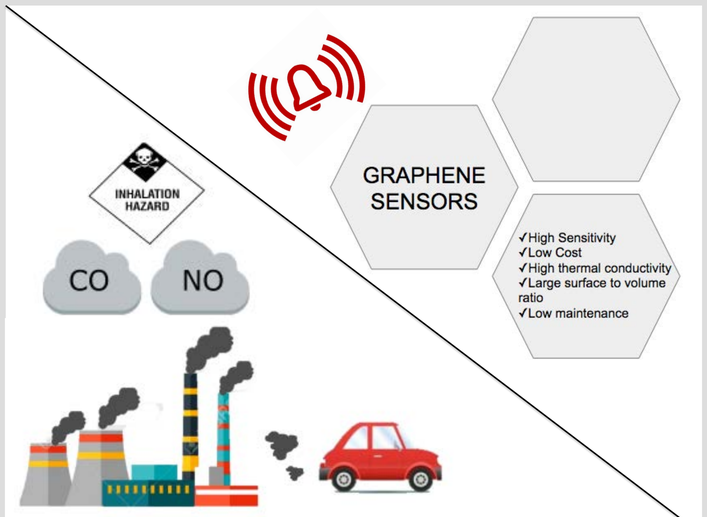
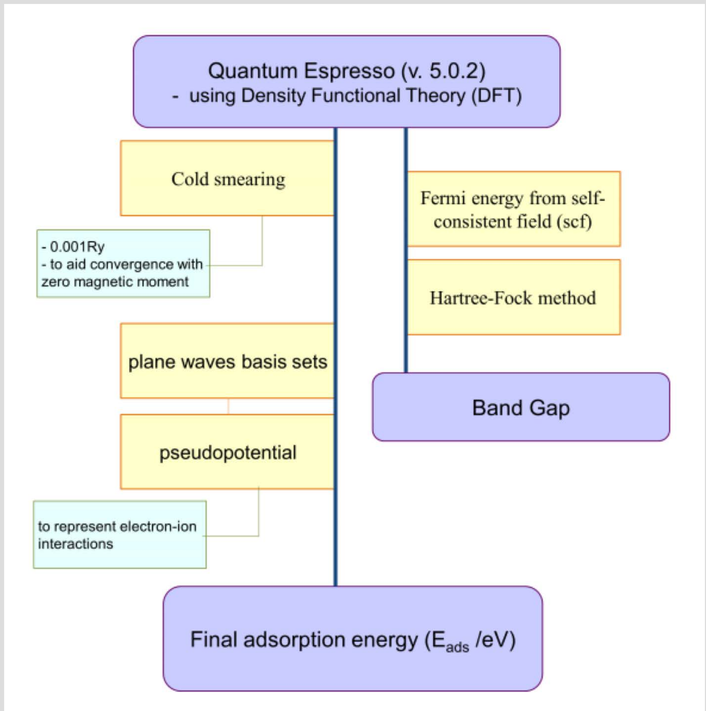
INTRODUCTION



A study of two-dimensional materials for gas sensors of toxic molecules is conducted. This is done by investigating adsorption thermodynamics and the effects of adsorption on the material's electronic properties. Interactions between graphene sheets and both Carbon Monoxide (CO) and Nitrogen Monoxide (NO) molecules are studied by running Plane-Wave Density Functional Theory (DFT) calculations using the open source software, Quantum Espresso. Calculations consider a range of factors: nature of the graphene sheet and number, position, orientation, and identity of the adsorbed molecules.

MATERIALS & METHODS



RESULTS

A. Final Adsorption Energy

Configuration		$E_{ads\ (N-O)}$ /eV	$E_{ads\ (C-O)}$ /eV
	0.1	**-4.56**	2.85
	1.1	-1.95	**-6.18**
	1.2	-1.95	**-6.18**
	1.hole	-0.12	-1.58
	1.holeB	-0.12	0.01

Smallest $E_{ads\ (N-O)}$ = most stable
Pristine graphene sheet is the most stable sensor in detecting 3% NO

Smallest $E_{ads\ (C-O)}$
A defect graphene sheet is the most stable sensor in detecting 3% CO

Figure 1(a) Final Adsorption energies (E_{ads}) of 3% NO-graphene and CO-graphene systems

All diagrams were self-drawn

Configuration		$E_{ads\ (N-O)}$ /eV	$E_{ads\ (C-O)}$ /eV
	0.1.2	-0.39	2.82
	0.1.3	-0.75	-0.04
	1.1.2	-2.94	**-10.52**
	1.1.3	-2.57	**-10.52**
	1.1.4	-2.48	-6.22
	1.1.5	**-3.47**	-3.42
	1.1.6	-2.84	-7.28
	1.2.4	-0.79	-0.89
	1.2.6	1.52	3.36
	1.2.7	-1.14	0.71
	1.3.6	-0.75	0.78
	1.3.7	14.5	2.27

$E_{ads\ (C-O)} < E_{ads\ (N-O)}$
Defect graphene is more sensitive in the detection of CO molecules

Figure 1(b) Final Adsorption energies (E_{ads}) of 6% NO-graphene and CO-graphene systems

All diagrams were self-drawn

B. Band Gap

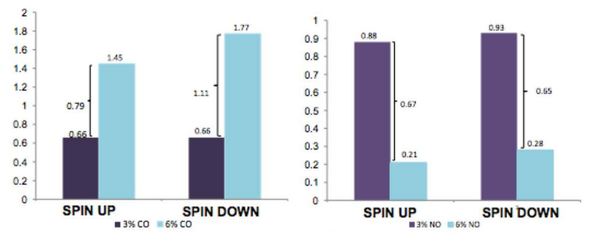
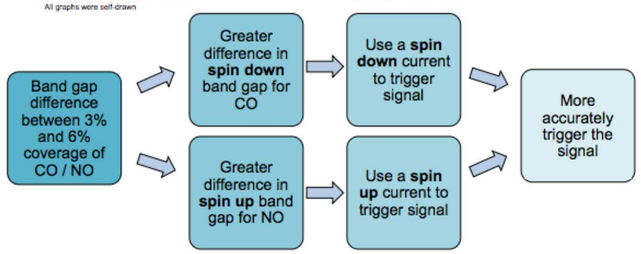


Figure 2(a): Comparison of the difference in band gap between 3% and 6% coverage of CO graphene system for spin up and spin down band gap

Figure 2(b): Comparison of the difference in band gap between 3% and 6% coverage of NO graphene system for spin up and spin down band gap

All graphs were self-drawn



CONCLUSIONS

Overall, it can be deduced that a defect graphene is more sensitive in the detection of CO molecules as shown by the small final absorption energy in both 3% and 6% coverage. Furthermore, the analysis in band gaps informs us that in order to have an accurate trigger of signal for 6% concentration, a spin down current should be used for CO molecules and a spin up current for NO molecules due to the greater difference in their band.

FUTURE WORK

1. Investigate the relationship between the orientation of the molecule and the interaction with graphene sheets.
2. Explore different material and its sensitivity in detecting toxic gas molecules.
3. To further investigate the relationship of different coverages and band gap.

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ACKNOWLEDGEMENTS

The authors gratefully thank Mr. Harman Johll, Dr. Jeong Choe, and Dr. Max McGee for their guidance as well as both Singapore's National Junior College and USA's Palo Alto Unified School District's (PAUSD) Advanced Authentic Research (AAR) program for their contributions of faculty, time and resources.