Partially-Oxidized Phosphorene-Based Sensors and Surface Oxidation Effects

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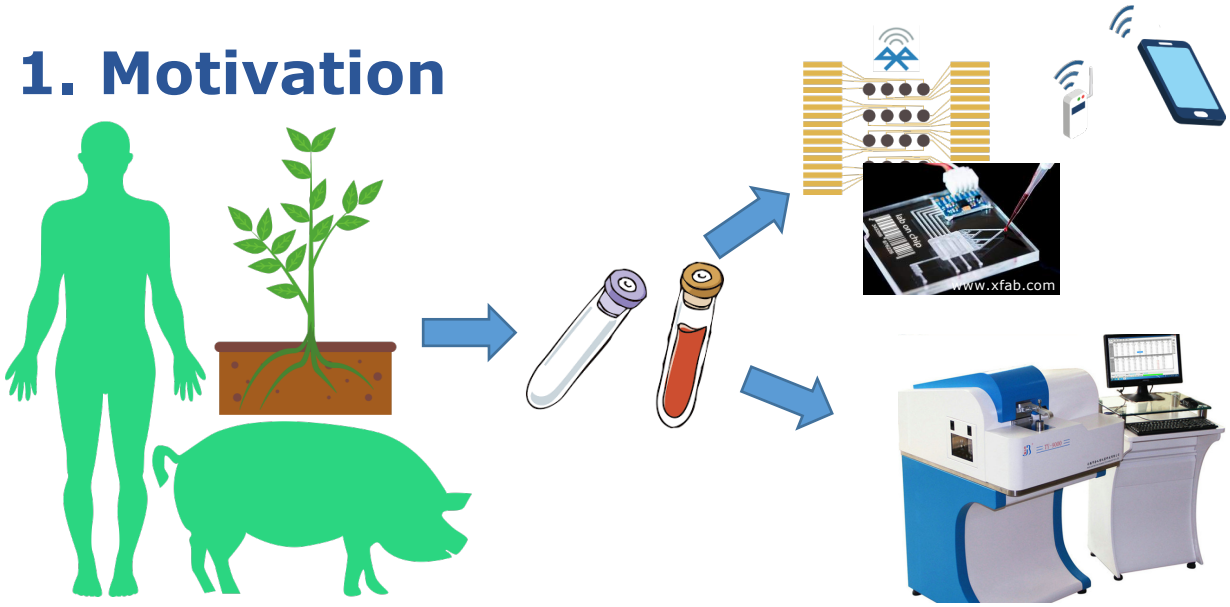
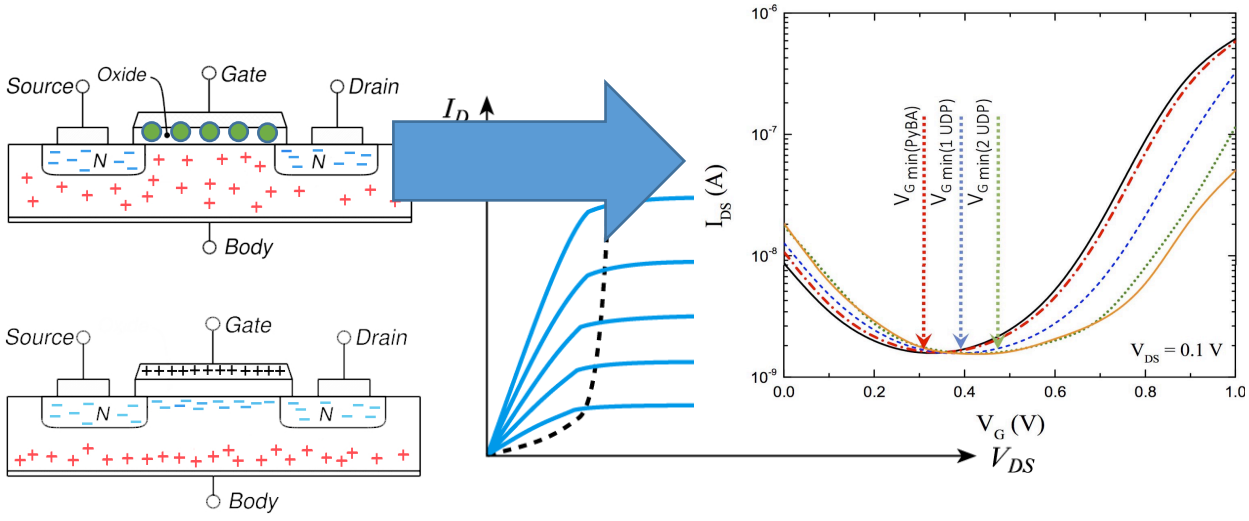
Outline

1. Motivation
2. Field-effect devices
3. Pristine and partially-oxidized phosphorene
4. Computational designs and characterization
5. Conclusions and future work

1. Motivation



2. Field-effect devices



3. Pristine and partially-oxidized phosphorene

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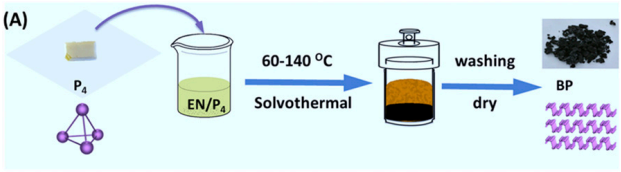
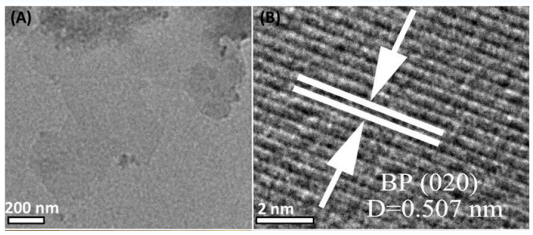
- Phosphorene: single-layer black phosphorus.
- Several approaches for fabricating few- and single-layer black phosphorus.
  - The material is unstable under ambient conditions.
  - Surface degrades within hours.

3. Pristine and partially-oxidized phosphorene



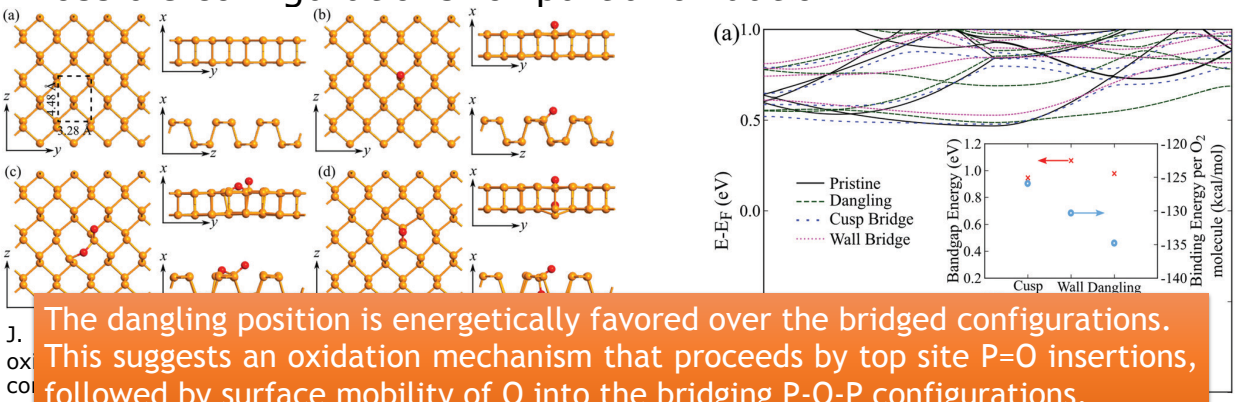


B. Tian et al., Proceedings of the National Academy of Sciences 115, 4345–4350 (2018).

- Novel approach for few-layer partially-oxidized black phosphorus.
  - Stability is significantly improved.
  - Oxygen content has little variation when compared with a 4-mo-aged sample.
  - Bandgap of obtained nanosheets was 1.19 eV.
  - P-O-P and O-P=O configurations are prevalently observed from X-ray photoemission spectroscopy (XPS) measurements.

4. Computational designs and characterization

- Possible configurations for partial oxidation.



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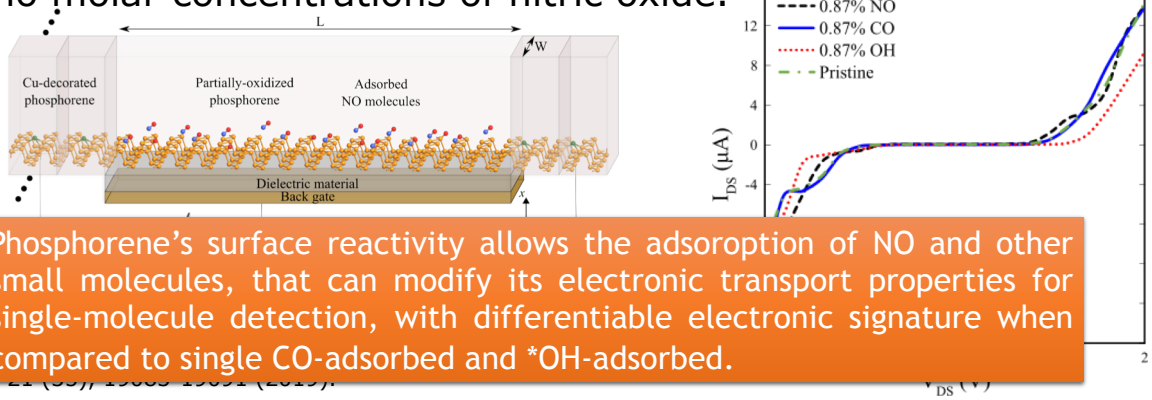
The dangling position is energetically favored over the bridged configurations. This suggests an oxidation mechanism that proceeds by top site P=O insertions, followed by surface mobility of O into the bridging P-O-P configurations.

4. Computational designs and characterization

- Partially-oxidized phosphorene sensor for the detection of sub-nano molar concentrations of nitric oxide.



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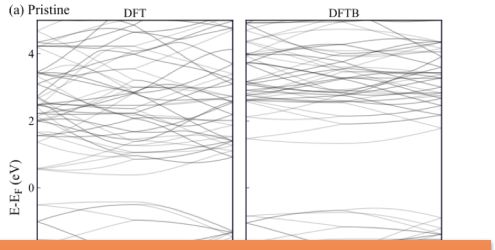
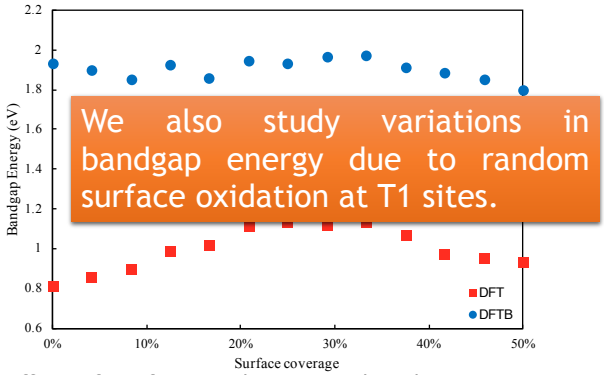
Phosphorene's surface reactivity allows the adsoroption of NO and other small molecules, that can modify its electronic transport properties for single-molecule detection, with differentiable electronic signature when compared to single CO-adsorbed and *OH-adsorbed.

4. Computational designs and characterization

- Comparison of electronic transport properties using DFT/DFTB.



DFTB calculations provide a very accurate bandgap prediction (~1.93 eV vs. ~0.81 eV with DFT).

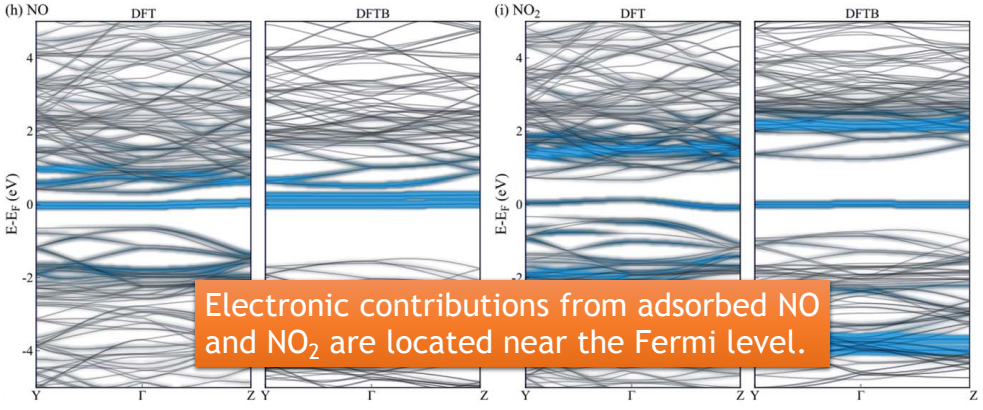


We also study variations in bandgap energy due to random surface oxidation at T1 sites.

J. M. Marmolejo-Tejada and A. Jaramillo-Botero, Effect of surface oxidation on the electronic transport properties of phosphorene gas sensors: a computational study, RSC Advances 10 (12), 6893-6899 (2020).

4. Computational designs and characterization

- Electronic contributions from adsorbed NO and NO_2 molecules.



Electronic contributions from adsorbed NO and NO_2 are located near the Fermi level.

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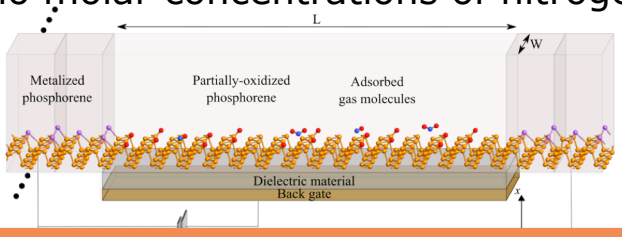
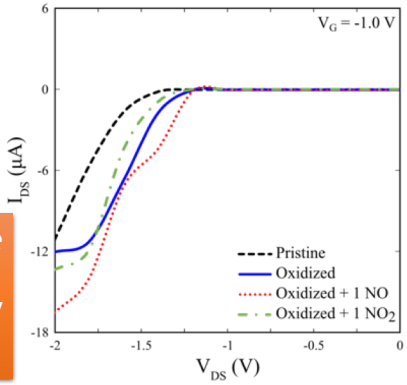
4. Computational designs and characterization

- Partially-oxidized phosphorene sensor for the detection of sub-nano molar concentrations of nitrogenated species.





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The device is capable of detecting single physisorbed NO and NO_2 molecules on the channel, with differentiable electronic signatures at V_G=-1V and V_{DS}=-2V, disregarding surface oxidation.

5. Conclusions and future work

- Partially-oxidized phosphorene could be practically used for gas sensing applications of nitrogen–oxygen moieties (adsorbed molecules whose electronic contribution is located near the systems' Fermi level).
  - Controlled oxidation of T1 sites on the phosphorene surface, up to 50% coverage, leads to preserved semiconducting properties, and sufficient binding sites for the potential detection of small organic molecules.
  - NO and NO_2 gas molecules bind to po-phosphorene's surface with favorable energy, and they can be selectively detected by means of a field-effect sensor.
- The presented designs provide basic architectural nodes for more complex bio-sensing logic circuits.
  - These may be embedded in mobile sensing devices for multiple applications.
- Next step: Experimental verification - Prototyping.

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Questions?

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