Application-driven Sensing Material Design for Volatile Organic Compound Sensors

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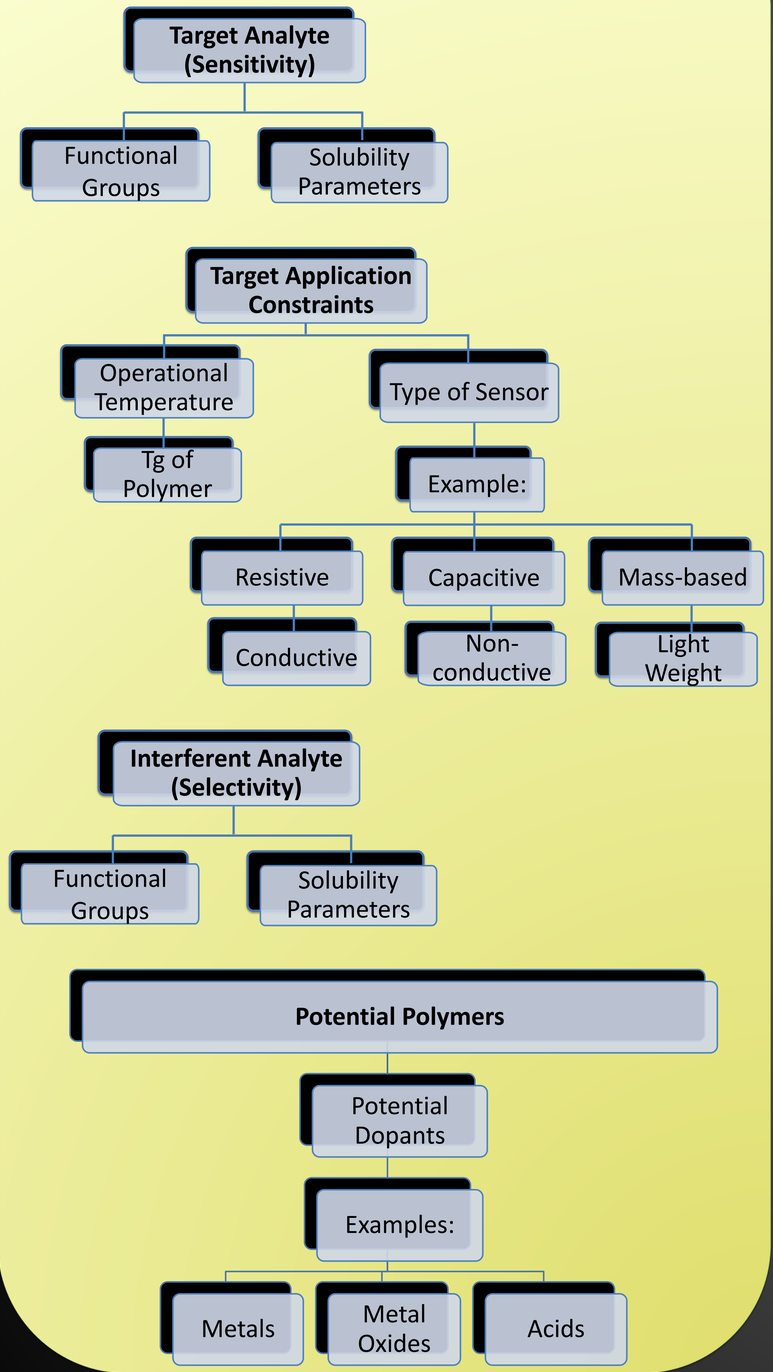
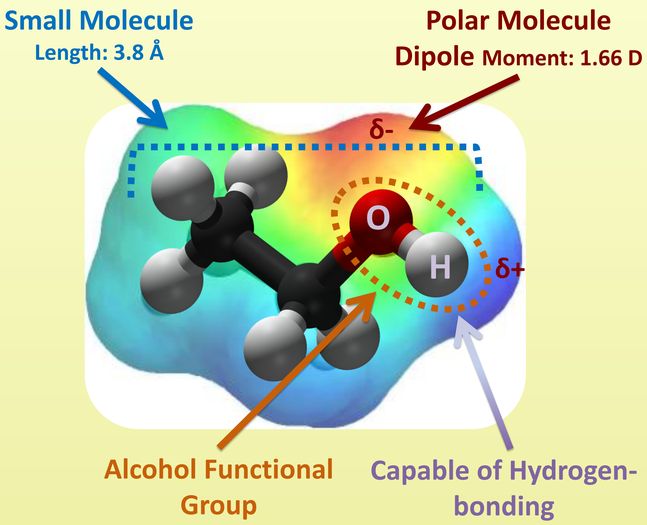
Material Selection



Target Analyte: Ethanol



- Polar backbone and/or functional groups
- Ideally capable of hydrogen-bonding
- Chains able to pack closely together to reduce interstitial spaces and thus, able to filter out larger analytes
- Potential dopants must be able to coordinate with both the polymer and ethanol

Application Requirements: Reduce Drinking and Driving

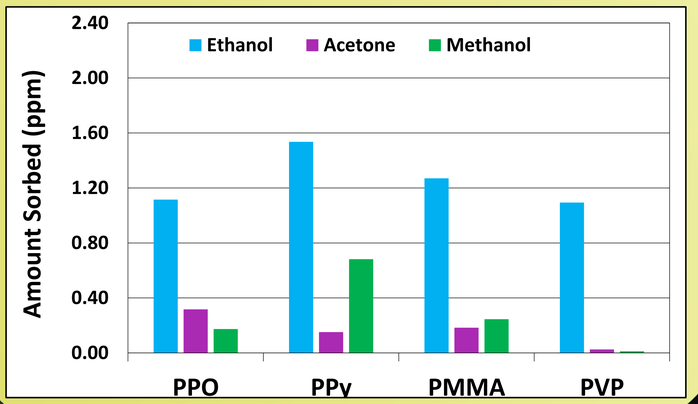
- Highly sensitive and selective detection of ethanol
- Operating Temperature up to 60 °C
  - Therefore, need a T_g above 60 °C
- Type of sensor: Unknown (in principle)
  - Therefore, no restrictions on conductivity
  - Best to choose some conductive and some non-conductive polymeric materials (flexibility for sensor selection)
- Common interferent: Acetone
  - Both acetone and ethanol are similar in size and polarity
  - But acetone is unable to hydrogen bond like ethanol

Potential Sensing Materials

Polymer	Glass Transition Temperature, T_g (°C)[1]	Hildebrand Solubility Parameter ($MPa^{1/2}$)[1]	Structure	Functional Groups
Poly (ethylene oxide) (PEO)	-43	19.9		-O-
Poly (vinyl acetate) (PVAc)	30	18.21		COOR
Polyamide (PA)	50	23.02		CNOR
Poly (lactic acid) (PLA)	57	21		COOR
Poly (ethylene terephthalate) (PETE)	67	21.9		COOR x2
Poly (vinyl alcohol) (PVA)	85	21.7		OH
Polyaniline (PANI)	100	22.2		NH
Poly (methyl methacrylate) (PMMA)	105	22.8		COOR
Poly (acrylic acid) (PAA)	106	19.2		COOH
Poly (vinyl pyrrolidone) (PVP)	128	25.6		CONR
Poly (2,6-dimethyl-1,4-phenylene oxide) (PPO)	215	19.6		-O-
Polypyrrole (PPy)	270	25.15		NH

Evaluation of Sensing Materials

- Four potential polymeric sensing materials were chosen
- Two conductive (PPO, PPy), two non-conductive (PMMA, PVP)
- All polymers were highly sensitive and selective for ethanol



Stewart, K. M. E. and A. Penlidis. "Designing Polymeric Sensing Materials: What are we Doing Wrong?" Polymers for Advanced Technologies **130**, 42 (2016) doi:10.1002/pat.3893.
Stewart, K. M. E. and A. Penlidis. "Evaluation of Polymeric Nanocomposites for the Detection of Toxic Gas Analytes" Journal of Macromolecular Science: Pure and Applied Chemistry **53**, 10 (2016) 610-618.
Stewart, K. M. E. and A. Penlidis. "Sensor Array for Volatile Organic Compounds based on Doped Poly (2,5-dimethyl aniline)" Macromolecular Symposia **370** (2016) 120-127.