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A novel composite film for detection and molecular weight determination of organic vapors

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SUPPORTING INFORMATION

Table S1: Detection limits, sensitivities, and ranges studied for different VOCs

VOC	Detection limit (mg/L)	Range studied (mg/L)	Sensitivity (Hz.L/mg)
acetone	0.0806	0.19-60.8	6.7
acetonitrile	0.0267	0.19-15.2	24.6
chloroform	0.1271	0.36-57.0	4.1
ethanol	0.1189	0.19-60.8	5.4
methanol	0.1611	0.19-61.1	3.8
toluene	0.0508	0.21-16.7	11.2

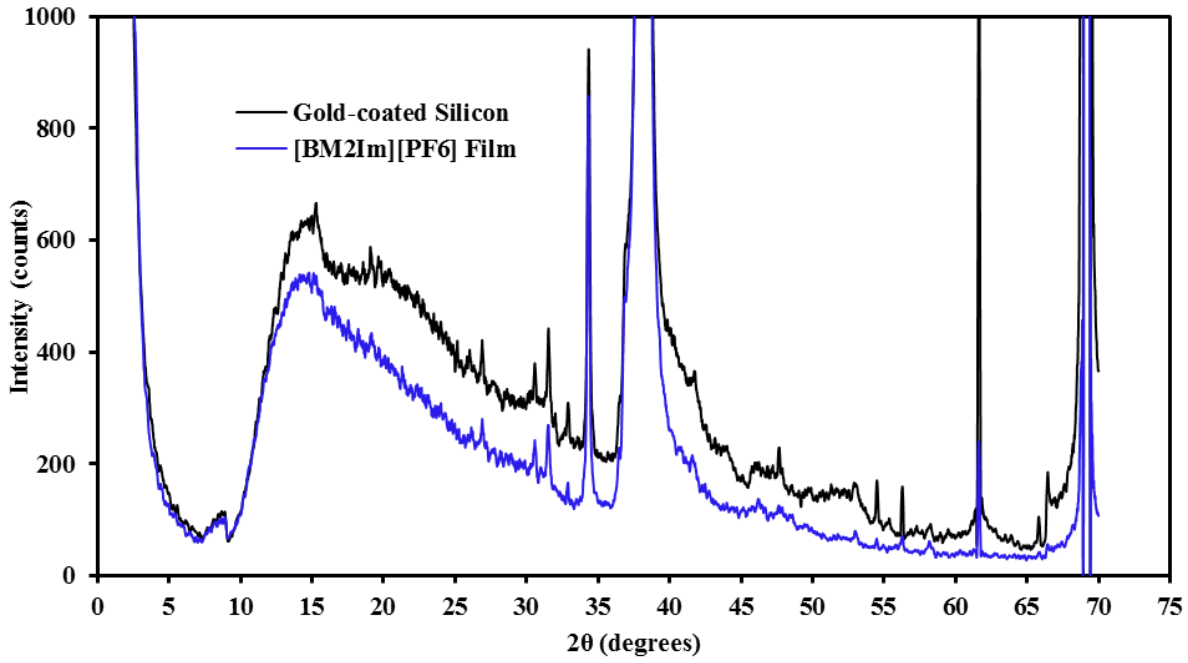

Fig. S1 XRD diffractograms of gold-coated silicon, and $[BM_2Im][PF_6]$ film deposited on the same substrate.

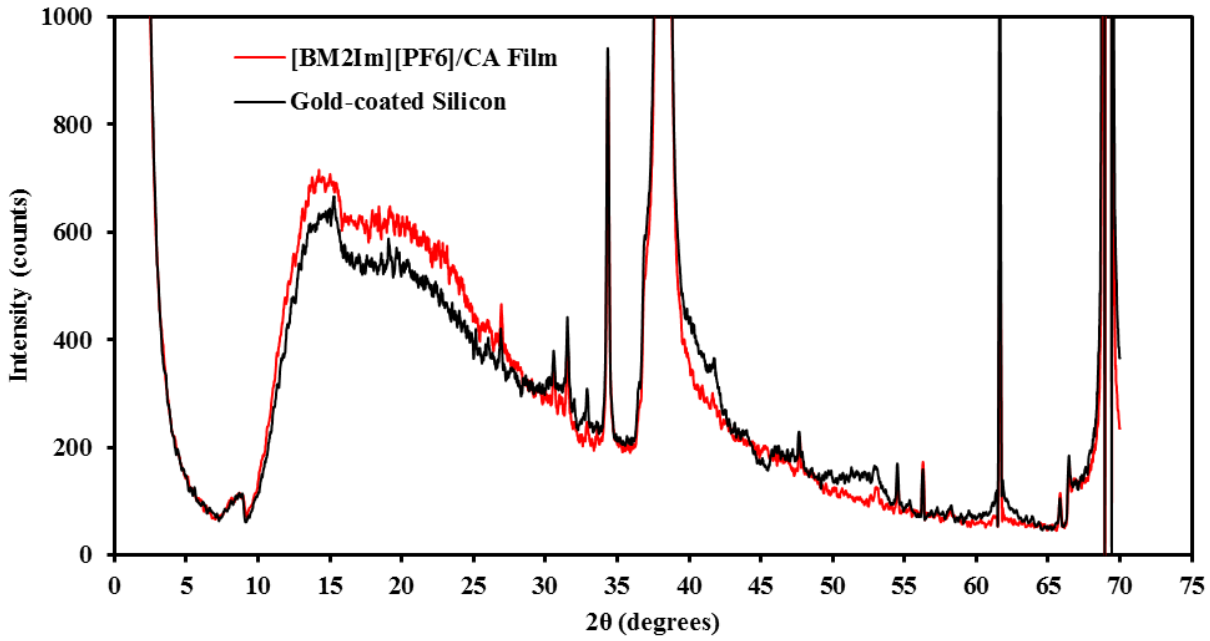

Fig. S2 XRD diffractograms of gold-coated silicon, and $[BM_2Im][PF_6]$-CA film deposited on the same substrate.

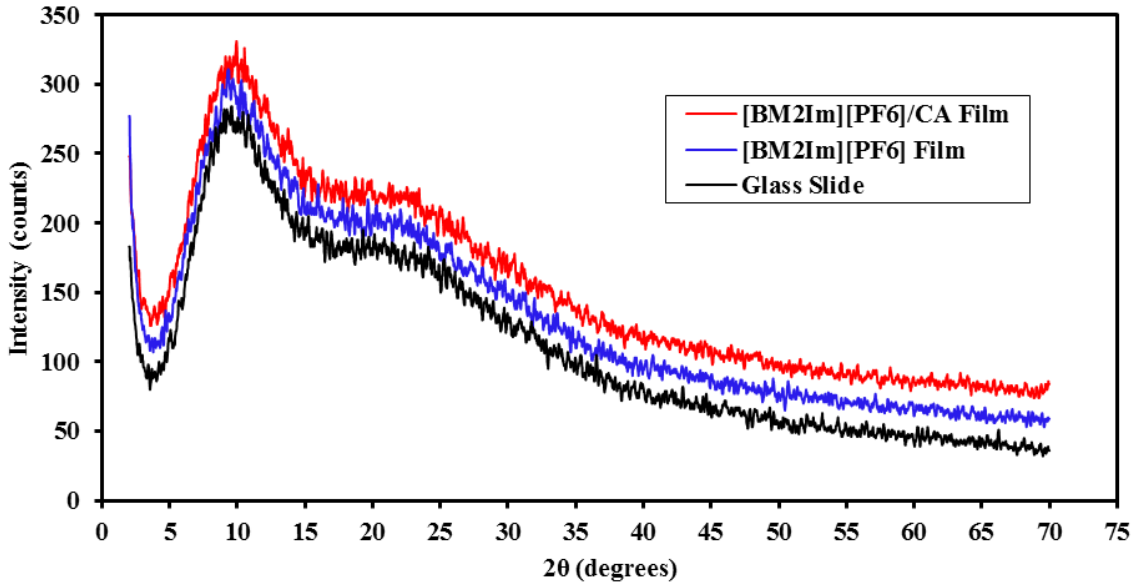

Fig. S3 XRD diffractograms of glass slide, $[BM_2Im][PF_6]$, and $[BM_2Im][PF_6]$-CA films deposited on the glass slide.

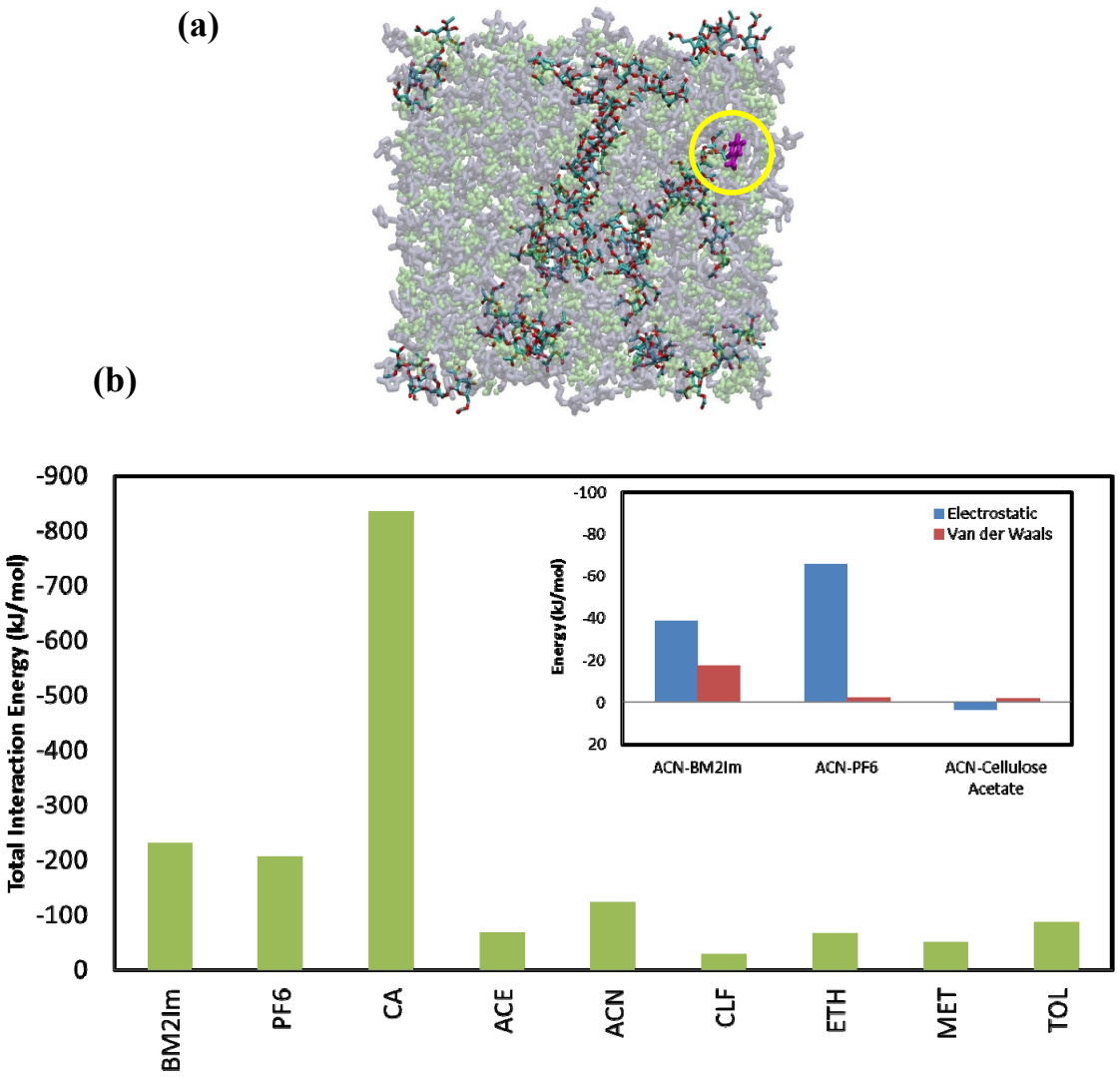

Fig. S4 (a) Simulation snapshot showing 500 $[BM_2Im][PF_6]$ pairs with 18 oligomers of CA and one molecule of VOC (toluene, circled in yellow). **(b)** Total interaction energy (i.e., sum of electrostatic and van der Waals interactions) exerted by all molecules present in the system to a single molecule of any given species. Shown in order (x-axis): a randomly chosen cation; a randomly chosen anion; a randomly chosen oligomer of cellulose acetate; and a molecule of analyte (in order: acetone, acetonitrile, chloroform, ethanol, methanol and toluene). The inset shows the electrostatic and van der Waals interactions experienced by a molecule of acetonitrile due to all the cations, anions and oligomers of cellulose acetate present in the system; the sum of all these energies give the total interaction energy experienced by the molecule of acetonitrile.

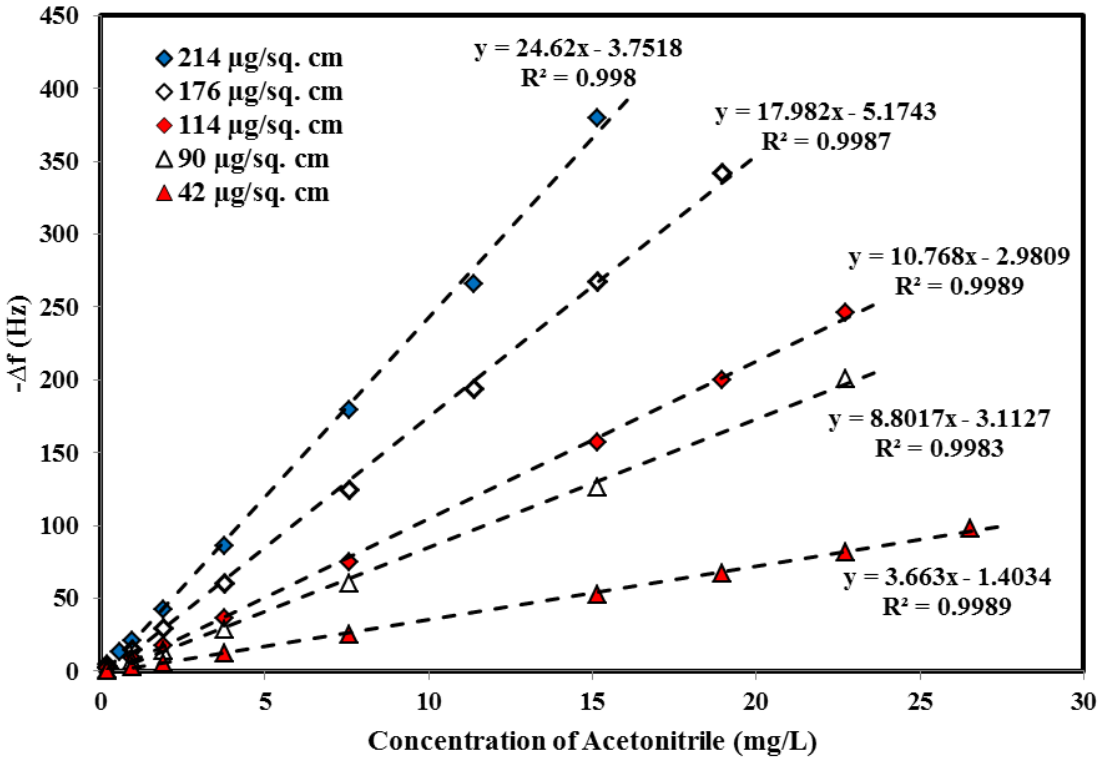

Fig. S5 Frequency shift versus acetonitrile vapor concentration for films containing different masses of the composite material. Legend shows the mass of the sensing material in each film.

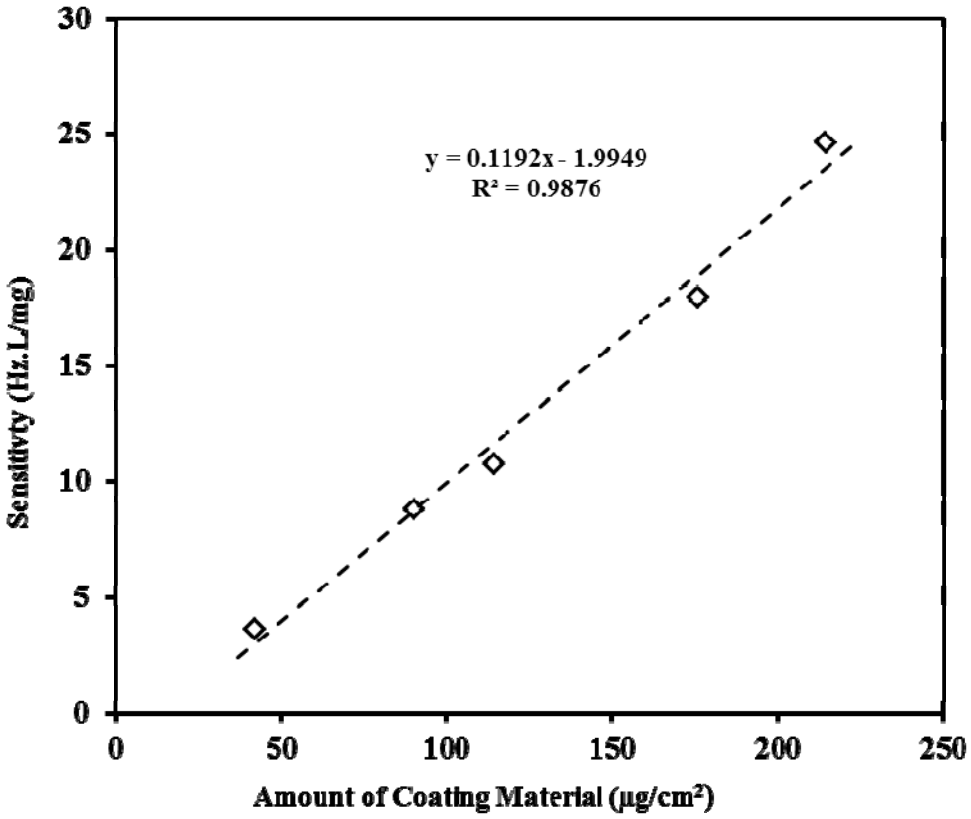

Fig. S6 Variation of sensitivity to acetonitrile vapors as a function of mass of sensing material.

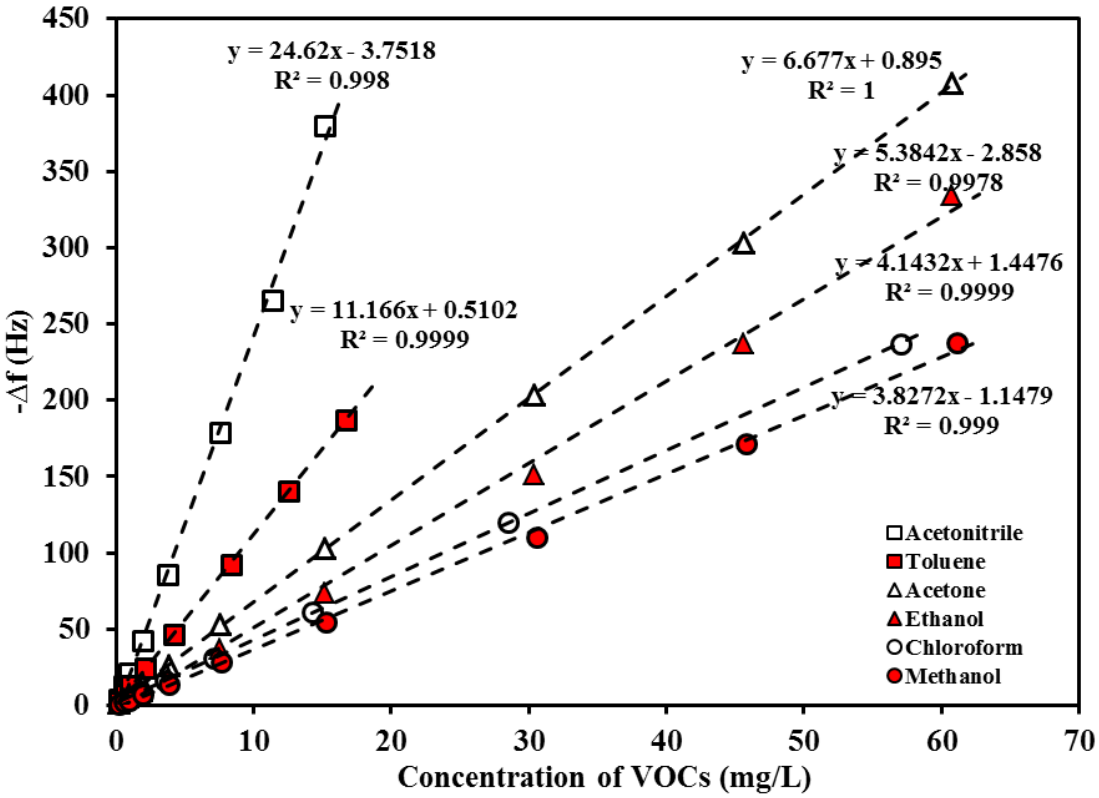

Fig. S7 Frequency shift as a function of vapor concentrations for various VOCs.

[In Fig. S4b, interaction energies are expressed in units of kJ/mol, while the slopes here are in units of Hz/(mg/L). For comparison, the slopes should be converted to moles of analyte absorbed per cm^2 for the same molar concentration of each vapor. Since Δf/(mg/L) is proportional to (moles/cm^2)/ (moles/L), the order remains the same].

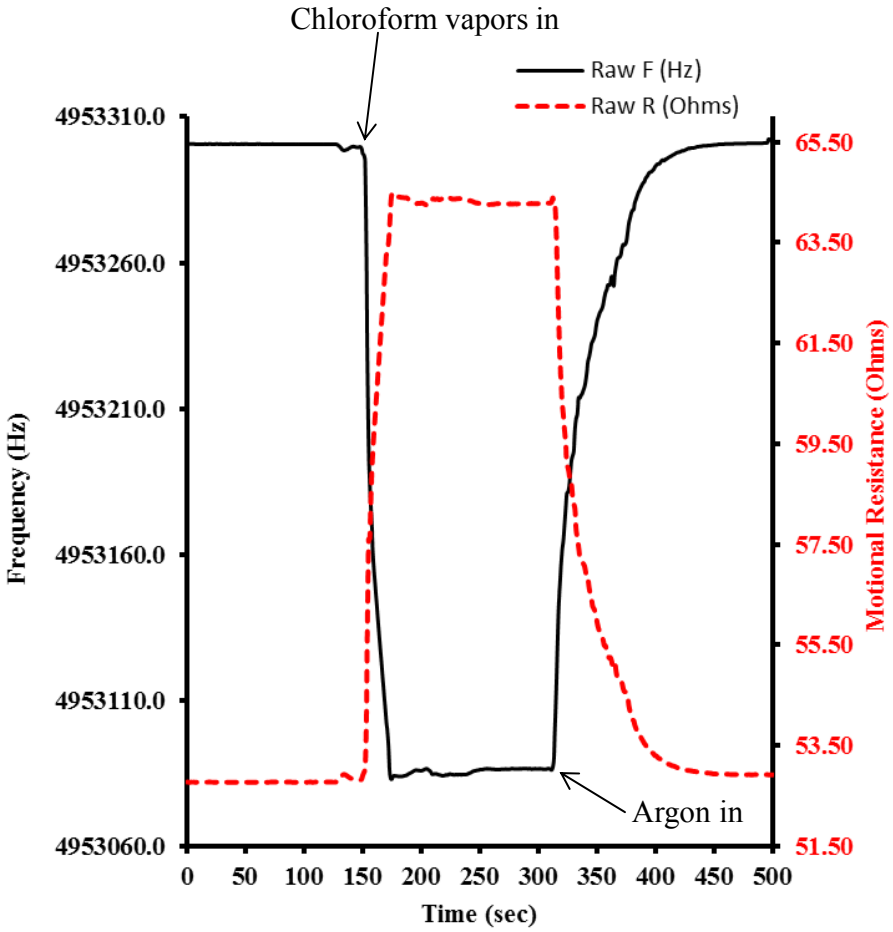

Fig. S8 Frequency and motional resistance responses of the sensor when PREMADE chloroform vapors are introduced into the measuring chamber.