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When few-layer black phosphorus meets small solvent molecules: reversible tuning of the optical and electrical properties

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Black phosphorus (BP) is becoming one of the most promising two-dimensional (2D) materials in view of its high-performance in (opto)electronics [1]. Solvents consisting of small molecules are often used for washing 2D materials or as liquid media for their chemical functionalization with larger molecules, disregarding their ability to change the opto-electronic properties of BP. Herein, we show that the electronic and optical properties of mechanically exfoliated few-layer BP are altered when physically interacting with common solvents. Significantly, charge transport analysis on field-effect transistors revealed that physisorbed solvent molecules induced a modulation of the charge carrier density which can be as high as 10¹²/cm² in black phosphorus, being comparable to traditional dopants F₄-TCNQ and MoO₃ [2] [3]. We have also found that the solvent physisorption determines a tuning of both hole and electron carrier mobility, enlargement of hysteresis in transfer curve and shift in Raman A_{1g} peak. We have as well proved that solvent molecules could effectively shift the work function of BP in a range of +0.16 eV to -0.15 eV. By combining experimental evidences with DFT calculations, we confirm that doping on BP by solvent molecules not only depends on charge transfer, but it is also influenced by trivial molecular dipole. Our results clearly demonstrate how an exquisite tuning of the optical and electrical properties of few-layer BP can be achieved through the simple physisorption of small solvent molecules which could serve as a guideline for both fundamental studies and more technological applications in opto-electronics. References

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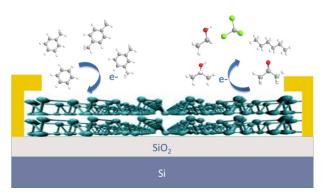


Figure 1: Tunable charge carrier density of few-layer black phosphorus *via* physisorption of small solvent molecules.