Supporting Information

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Electronic Transport in 2D-Based Printed FETs from a Multiscale Perspective

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S1 Multi-scale conductance calculations

Figure S1: a) Hamiltonian of the overlapped structure with the diagonal blocks explaining the top and bottom flakes band-structures, and the off-diagonal blocks determining the coupling between both layers b) Construction of the extended Hamiltonian with arbitrary sizes of the overlapping and single-flake regions. The triangles represents the connections between adjacent cells along the structure.
S2 Charge density difference calculations

The charge density difference (CDD) (\(\Delta \rho\)) for graphene and MoS\(_2\) bilayer structures was obtained from the equation \(\Delta \rho = \rho_{\text{bilayer}} - \rho_{\text{top}} - \rho_{\text{bot}}\) where \(\rho_{\text{bilayer}}\), \(\rho_{\text{top}}\) and \(\rho_{\text{bot}}\) are the total charge density of the bilayer structure (see Fig. 2 (a, b) bottom), of the top layer only and the bottom layer only, respectively, calculated by means of the Quantum Espresso suite S[1]. The CDD highlights the charge redistribution in the bilayer graphene with respect to the monolayer structure.
S3 Mobility experimental validation

We have compared the extracted effective mobility as a function of the thickness with the measurements after annealing in Ref. S[2], keeping the same unintentional doping and mobility values as is the main manuscript. The results in the range of thicknesses considered in this work are shown in Fig. S2, showing a good agreement and thus supporting the in-plane mobility value considered within the study.

Figure S2: Extracted mobility for graphene as a function of the channel thicknesses compared with experimental results obtained in Ref. S[2] for after annealing samples.
S4 Conductance calculation

Conductance is calculated by the Landauer-Buttiker linear response theory as

\[ G = \frac{2q^2}{h} \int_{E_{\text{min}}}^{E_{\text{max}}} T(E) \frac{\partial f}{\partial E} \left( \frac{E - E_F}{k_B T} \right) dE \]  

(1)

where \( q \) is the elementary charge, \( h \) is Planck’s constant, \( f \) is the Fermi-Dirac function, \( T(E) \) the transmission coefficient as a function of energy and \( E_F \) the Fermi level. The analytical function used for the fitting of graphene conductance ratio is reported hereafter together with the fitting parameters

\[ g_G = -a \cdot \exp \left( -\frac{(x - b)^2}{c^2} \right) + d + e \cdot x \]  

(2)

with \( a = 0.1445, b = 0.0073 \) eV, \( c = 0.1002 \) eV, \( d = 0.6004, e = 0.0566 \) eV\(^{-1} \) and \( x \) being the Fermi level.

Similarly, for MoS\(_2\):

\[ g_{\text{MoS}_2} = a + b \cdot x + c \cdot (x - d)^2 + e \cdot x^3 + f \cdot x^4 + g \cdot x^5 \]  

(3)

with \( a = 19.507, b = 45.313 \) eV\(^{-1} \), \( c = 551.36 \) eV\(^{-2} \), \( d = 0.371 \) eV, \( e = -414.17 \) eV\(^{-3} \), \( f = 154.76 \) eV\(^{-4} \), \( g = -23.06 \) eV\(^{-5} \) and \( x \) being the Fermi level.
S5 Channel mobility extraction

We have extracted $\mu_{\text{eff}}$ for the whole network-FET applying the direct transconductance method S[3, 4], in order to mimic the typical experimental extraction procedure, that is by the expression

$$\mu_{\text{eff}} = \frac{g_m}{C_{\text{ins,spec}}} \cdot \frac{L}{W} \cdot \frac{1}{V_{DS}} \quad (4)$$

where $g_m = \partial I_{DS}/\partial V_G$ is the transconductance calculated at $V_D + V_{DS}$ for graphene and at $V_{th} + V_{DS}$ for MoS$_2$, $C_{\text{ins,spec}} = \varepsilon_r \varepsilon_0 / t$ is the specific insulator capacitance and $L/W$ the device aspect ratio. The analytical expressions of mobility guides for the eye have been obtained with the following expressions for graphene and MoS$_2$, respectively.

$$\mu_G = a \cdot x + b \quad (5)$$
$$\mu_{\text{MoS}_2} = c \cdot x + d \quad (6)$$

where $x$ is the filling factor, $a = 37.23 \text{ cm}^2/\text{Vs}$, $b = -11.52 \text{ cm}^2/\text{Vs}$, $c = 2.96 \text{ cm}^2/\text{Vs}$ and $d = -0.93 \text{ cm}^2/\text{Vs}$.
S6  Sheet resistance calculation

For thin-film materials, sheet resistance is generally the key parameter which allows comparison and evaluation of material quality and it is defined as:

\[ R_{sheet} = \frac{W}{L} \cdot \frac{dV}{dI_{DS}} \]  

(7)

where \( dV/dI_{DS} \) is the inverse of the output characteristic current slope and \( W/L \) the aspect ratio reciprocal and thickness, which does not appear in the formula, is considered constant for the whole structure. The analytical expressions of resistance guides for the eye have been obtained with the following expressions for graphene and MoS\(_2\), respectively:

\[ R_G = a \cdot \exp(-b \cdot (x + c)) + d \]  

(8)

\[ R_{MoS_2} = \frac{h}{x^j} + k \]  

(9)

where \( x \) is the filling factor, \( a = 5.68 \cdot 10^8 \ \Omega/\square \), \( b = 18.65 \), \( c = 0.3 \), \( d = 431.7 \ \Omega/\square \) for graphene and \( h = 4.28 \cdot 10^4 \ \Omega/\square \), \( j = 6.63 \), \( k = 9.56 \cdot 10^6 \ \Omega/\square \) for MoS\(_2\).
Figure S3: Transfer characteristics normalized by the device width for 30-samples simulations as a function of the flakes filling factor $FF$ and of channel thickness in linear scale for graphene printed FETs. The solid line indicates the mean value and the shaded areas include the standard deviation.
## Table of quantities

| Quantity                        | Abbreviation | Short description                                                      | Value          |
|--------------------------------|--------------|------------------------------------------------------------------------|----------------|
| Filling factor                 | FF           | Volume occupied by the flakes with respect to the overall channel volume | 0.3-0.7        |
| Graphene in plane mobility     | $\mu_{Gr}$   |                                                                        | 200 cm$^2$/Vs  |
| MoS$_2$ in plane mobility      | $\mu_{MoS_2}$|                                                                        | 2 cm$^2$/Vs    |
| Effective mobility             | $\mu$        | Extracted effective mobility from the simulations (either for graphene and MoS$_2$ based devices) | 1-16 cm$^2$/Vs for graphene; 0-1 cm$^2$/Vs for MoS$_2$ |
| Flake lateral dimension        | L            | Average dimension of the single flake                                  | 150 nm         |
| Flake thickness                |              | thickness of the single flake                                         | 0.5 nm         |
| Channel length                 |              | Length of the whole printed device channel                            | 3 \mu m        |
| Channel width                  |              | Width of the whole printed device channel                             | 1 \mu m        |
| Channel thickness              |              | Thickness of the whole printed device channel                         | 25-150 nm      |
| Sheet resistance               | $R_{\text{sheet}}$ | Sheet resistance of the whole printed device |               |

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