Electronic Supplementary Material (ESI) for RSC Advances.

Tunable Ohmic van der Waals-type Contacts in Monolayer C_3N Field-effect Transistors

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Table S1. Lattice constants of ML C_3N and independent 2D metal electrodes (graphene, $Ti_2C(OH/F)_2$, and $Zr_2C(OH/F)_2$) and bulk metals (Au, Ni, Pd, and Pt).

Lattice parameter										
	ML C_3N	graphene	Zr_2CF_2	Ti_2CF_2	$Ti_2C(OH)_2$	$Zr_2C(OH)_2$	Ni	Au	Pd	Pt
a (Å)	4.86	2.46	3.05	3.05	3.04	3.04	2.47	2.86	2.77	2.71
b (Å)	4.21	2.46	3.05	3.05	3.04	3.04	2.47	2.86	2.77	2.71

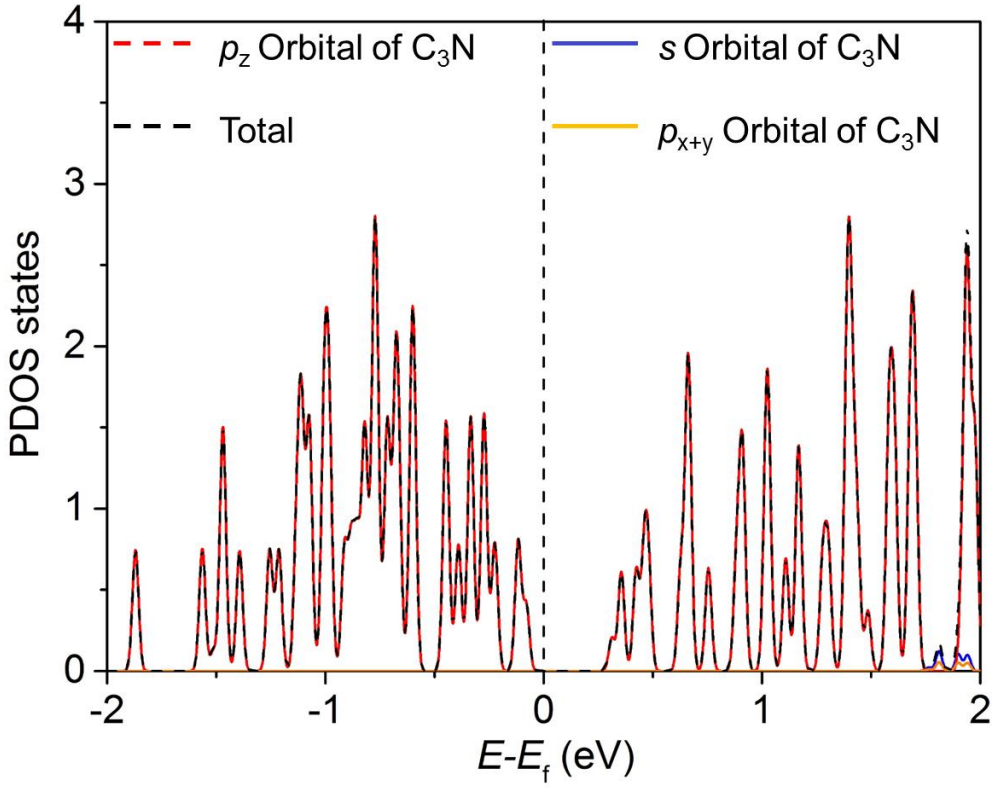

Figure S1. PDOS of the pristine ML C_3N. The red dash line, the blue line, the yellow line, and the black dash line are the DOS of the p_z orbital, s orbital, p_{x+y} orbital, and the total orbital of the ML C_3N, respectively. The Fermi level is set at zero energy and denoted by the lateral black dashed lines.

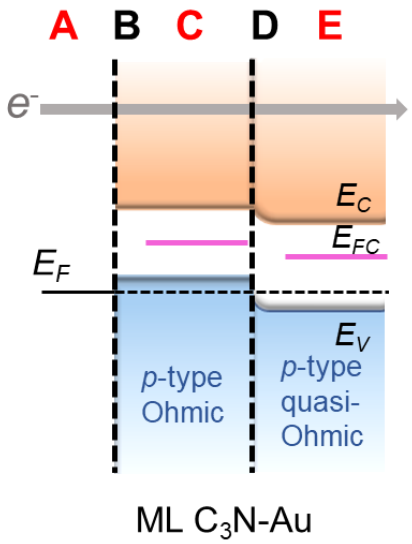

Figure S2. A possible band diagram in terms of the quantum transport calculations of ML C_3N FETs with Au in the zigzag direction. E_C and E_V are the conduction and valence band edges of the ML C_3N, respectively. E_F and E_{FC} denote the Fermi level of the ML C_3N-electrode junctions and the band gap center of the channel ML C_3N, respectively.