Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Electric-field-tunable molecular adsorption on germanane

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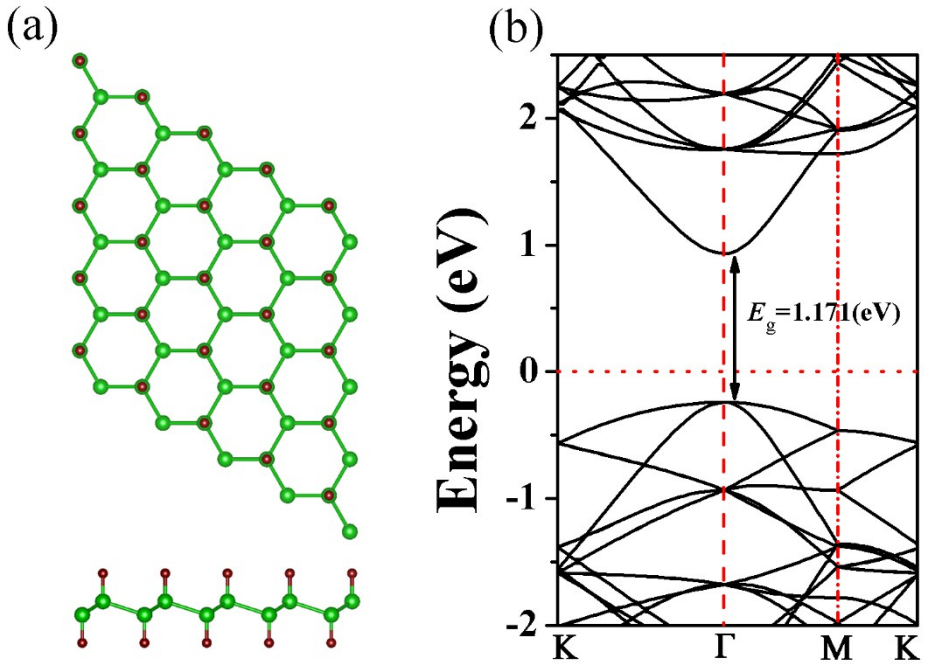

Fig. S1 (a) The top and side views of germanane. The green and brown spheres represent Ge and H atom, respectively. (b) The band structures of germanane. The Fermi level is set to 0 eV.

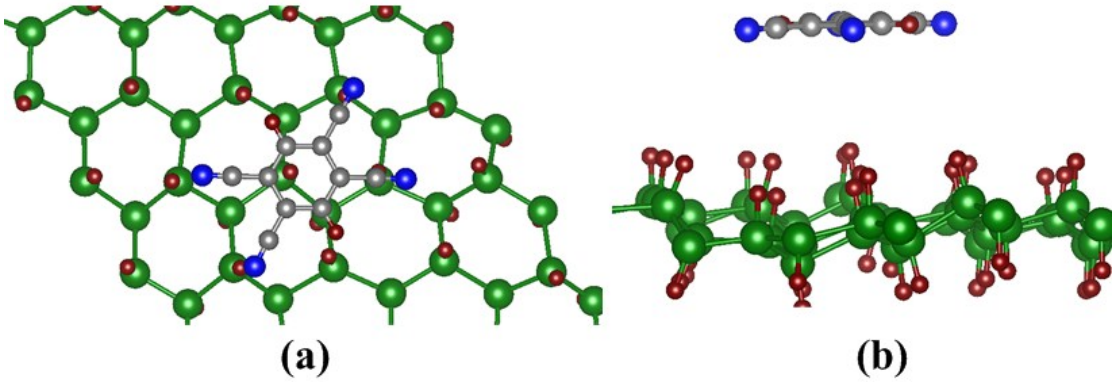

Fig. S2 (a)-(b)The top view and side view of germanane/TCNB under 300k for 10 ps.

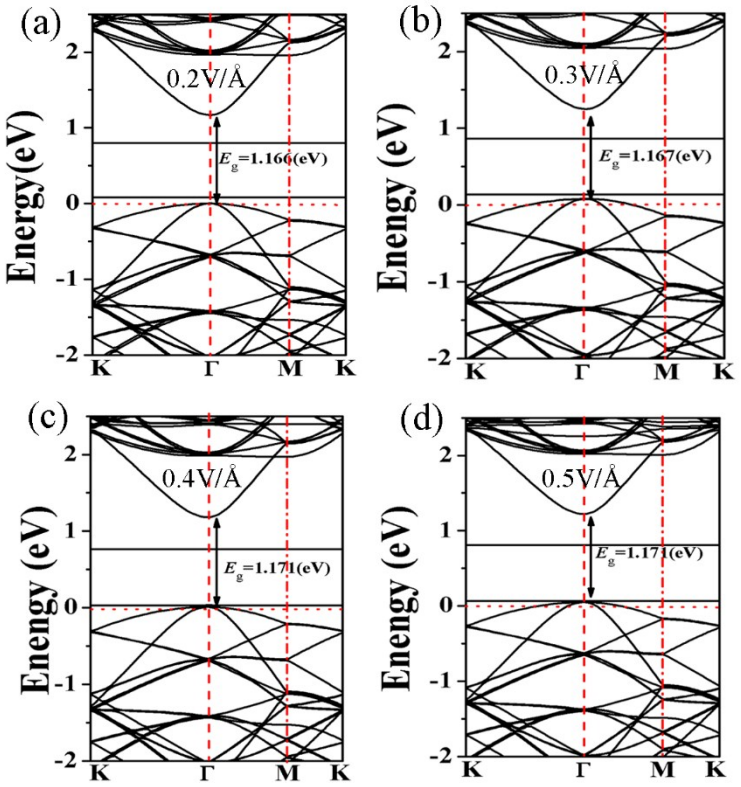

Fig. S3 (a)-(d) The band structures of germanane/TCNB under E-field of 0.2 V/Å, 0.3 V/Å, 0.4 V/Å and 0.5 V/Å, respectively. The Fermi level is set to 0 eV.

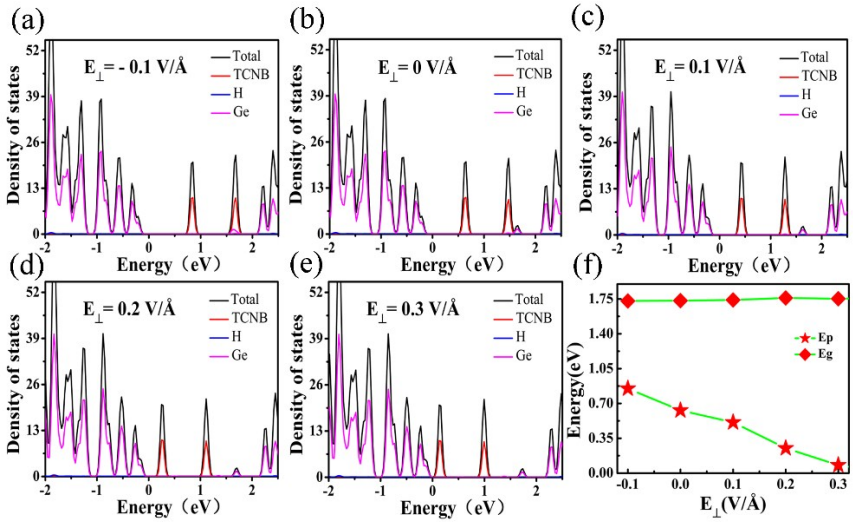

Fig. S4 The projected density of states for germanane/TCNB and the evolution of Ep under different E-field by using HSE06 method

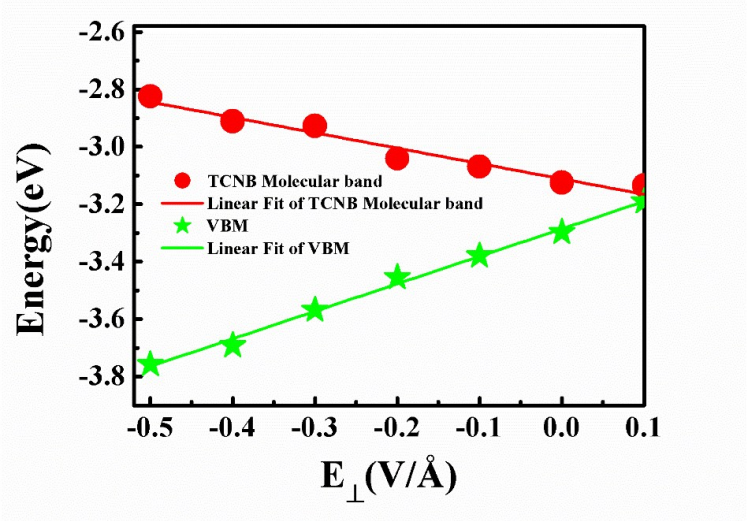

Fig. S5 The energies for VBM at Γ-point and the empty band minimum of TCNB with respect to Fermi level in conduction bands as a function *vs* E-field ranged from -0.5V/Å to 0.1 V/Å.