Graphdiyne-metal contacts and graphdiyne transistors

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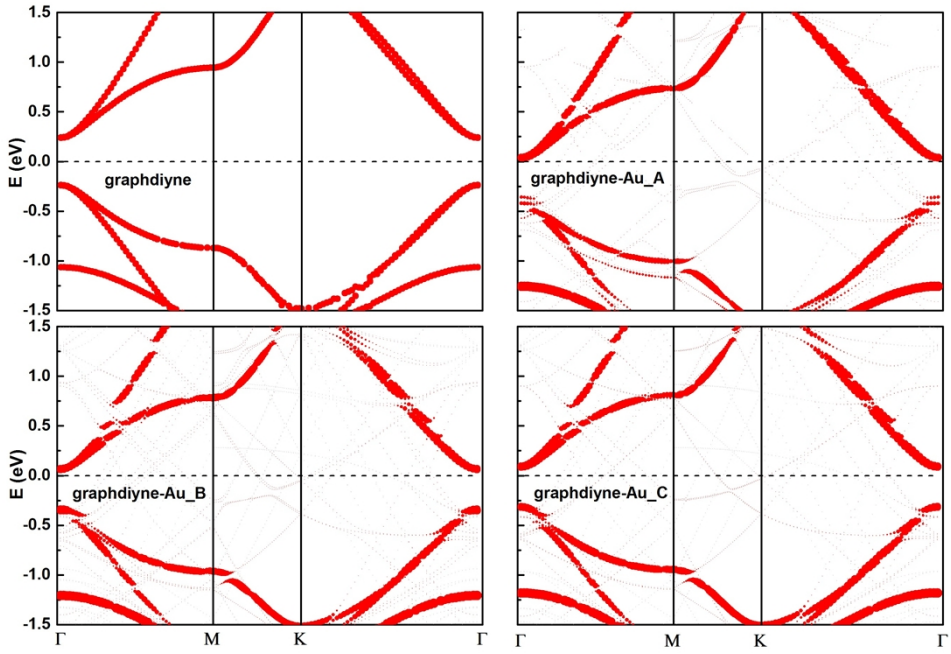

Fig. S1 Band structure of pure graphdiyne and graphdiyne adsorbed on Au surface of three kind configurations (graphdiyne-Au_A, B, C present the configuration of the center of the carbon hexagon of graphdiyne on the top of metal atoms of A, B, and C layer, respectively). The Fermi level is set at zero energy. Gray line: the bands of adsorbed systems; red line: the bands of graphdiyne.

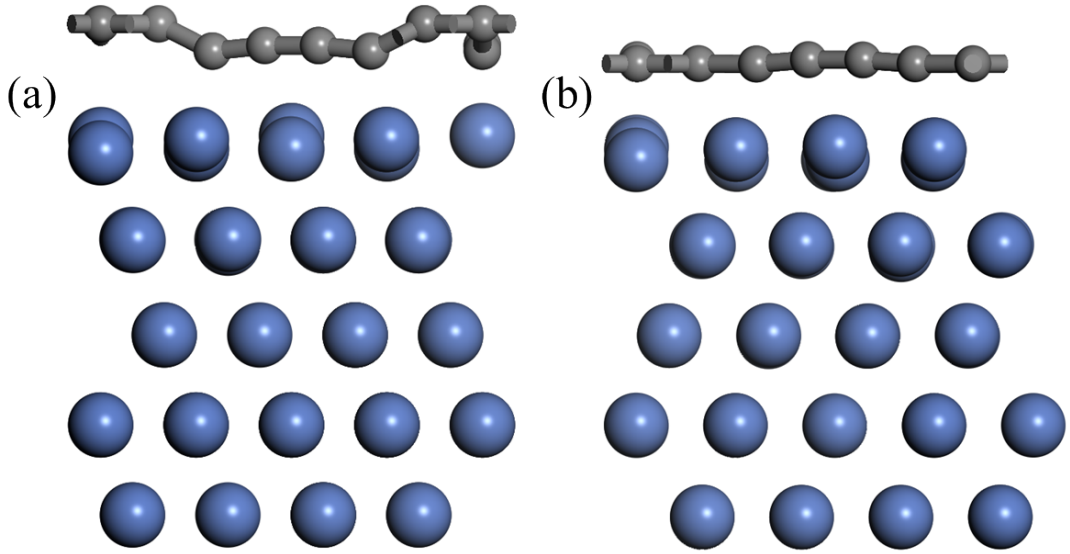

Fig. S2 Comparison of the optimized structure of the system (a) Ni surface (blue balls) adjusted to graphdiyne (gray balls) and (b) graphdiyne adjusted to Ni surface.

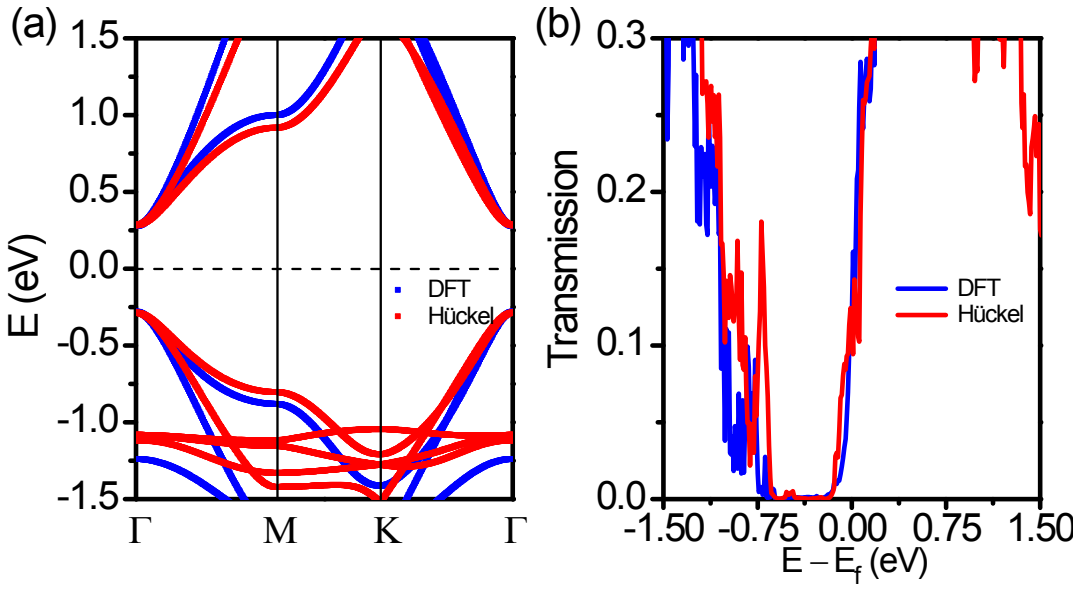

Fig. S3 Comparison of (a) the band structure of graphdiyne and (b) the transmission spectra of the 6 nm-channel-length graphdiyne FET (V_g = 0 and V_{bias} = 0) calculated by DFT (blue) and SE (red) methods.