Supplementary Materials

Acheving High Quantum Capacitance Graphdiyne through Doping and Adsorption

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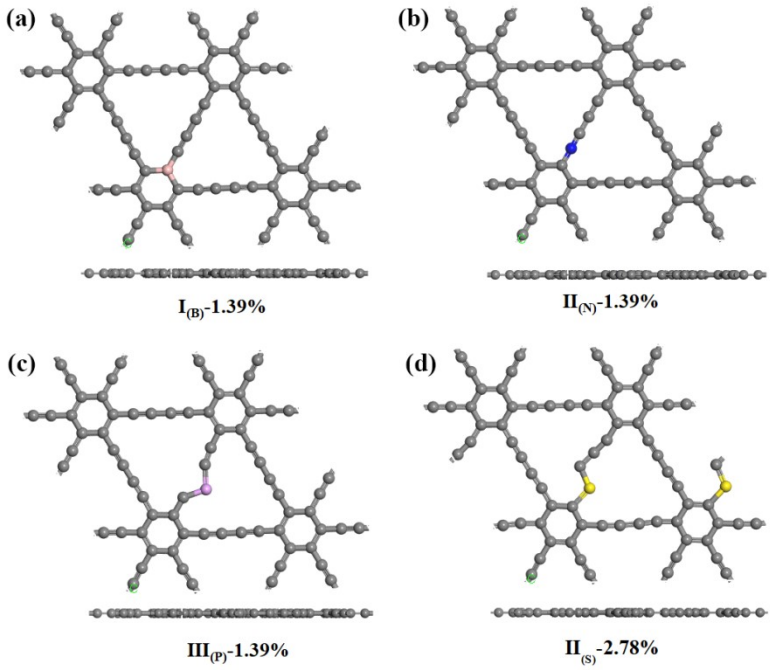

Fig. S1 Structure of B/N/P/S doped GDY optimized at the lowest formation energy

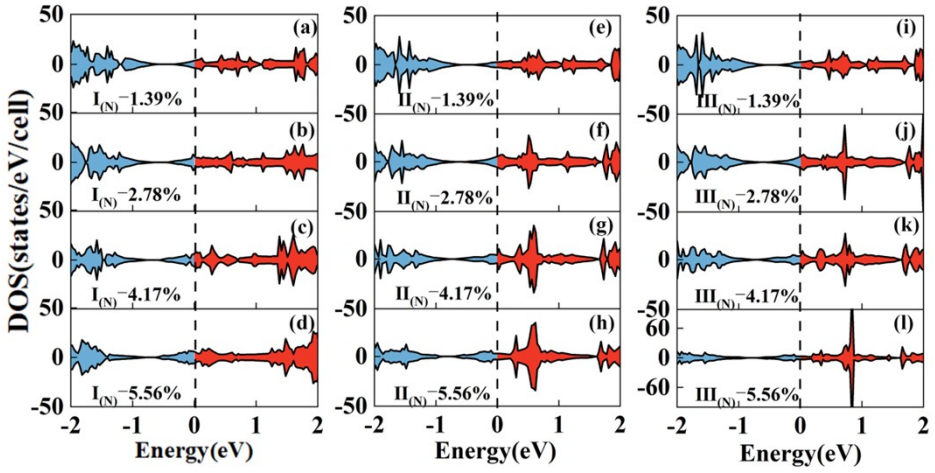

Fig. S2 Density of states maps of N atoms with doping concentrations of 1.39%, 2.78%, 4.17% and 5.56% at positions I, II, and III, respectively.

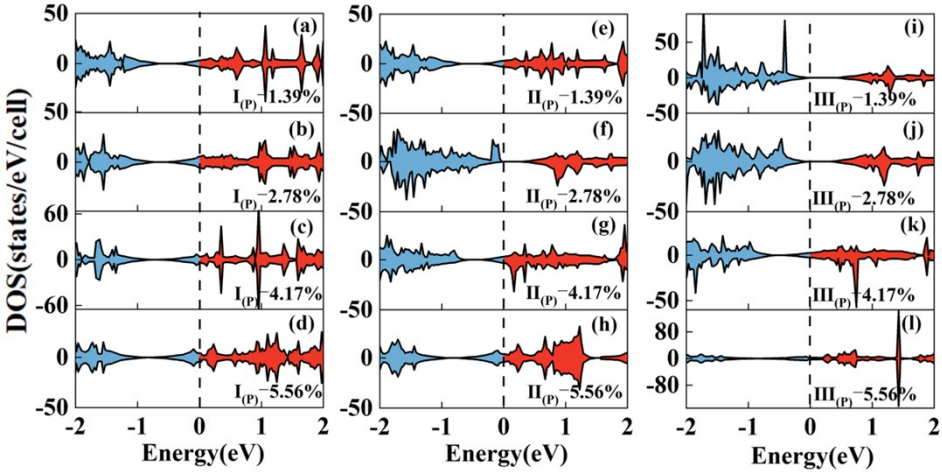

Fig. S3 Density of states maps of P atoms with doping concentrations of 1.39%, 2.78%, 4.17% and 5.56% at positions I, II, and III, respectively.

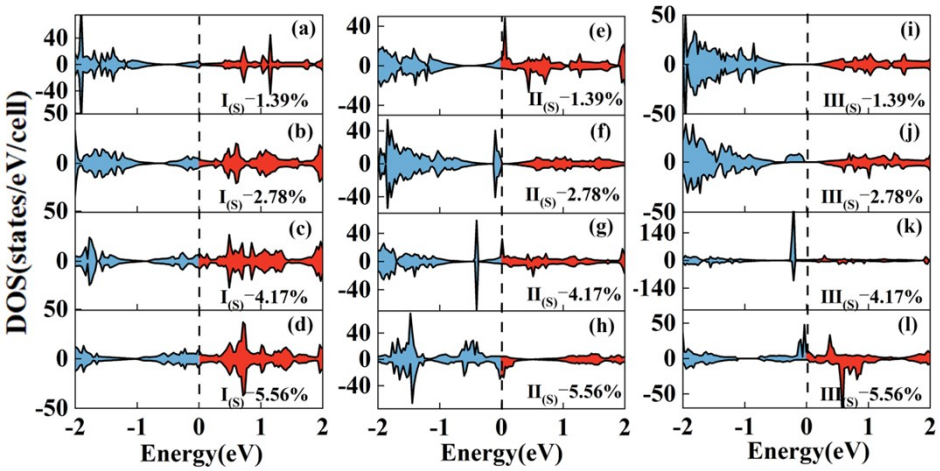

Fig. S4 Density of states maps of S atoms with doping concentrations of 1.39%, 2.78%, 4.17% and 5.56% at positions I, II, and III, respectively.

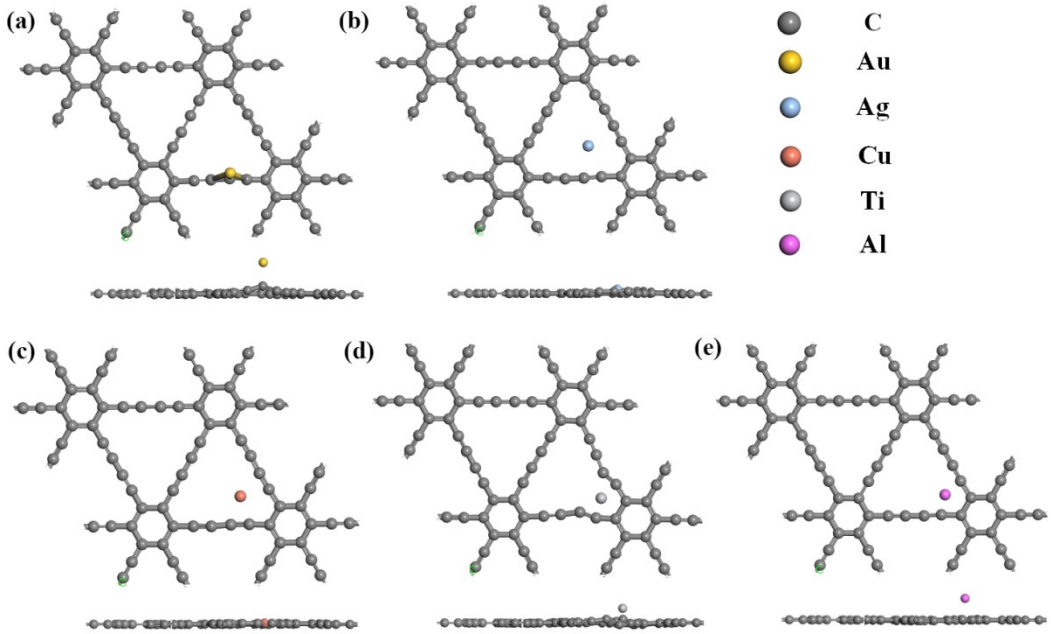

Fig. S5 Optimized structure diagram of metal atom adsorbed at V positions

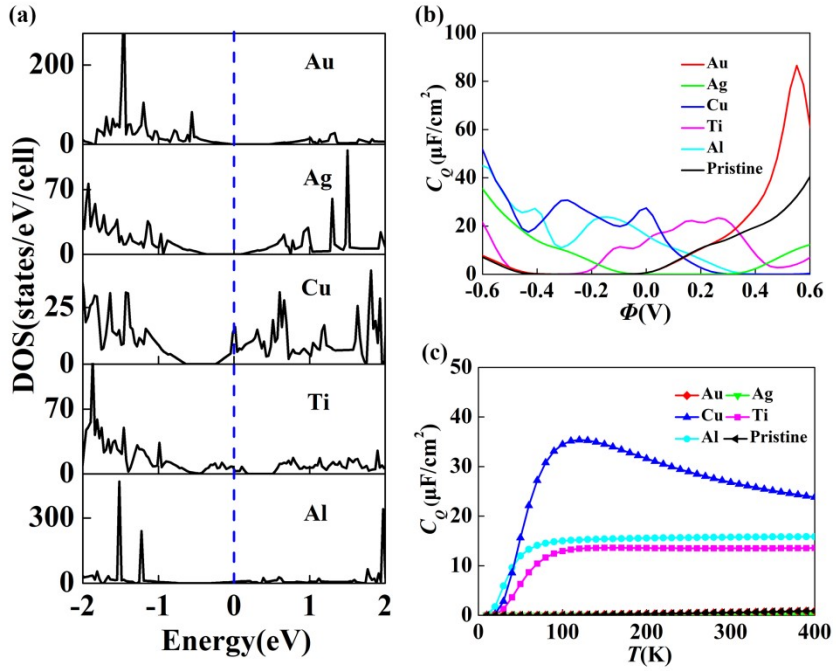

Fig. S6 (a) Density of electronic states of Au, Ag, Cu, Ti, and Al atoms adsorbed at the IV

position; C_Q as a function of (b) potential (-0.6~0.6V) and (c) temperature (0~400 K).

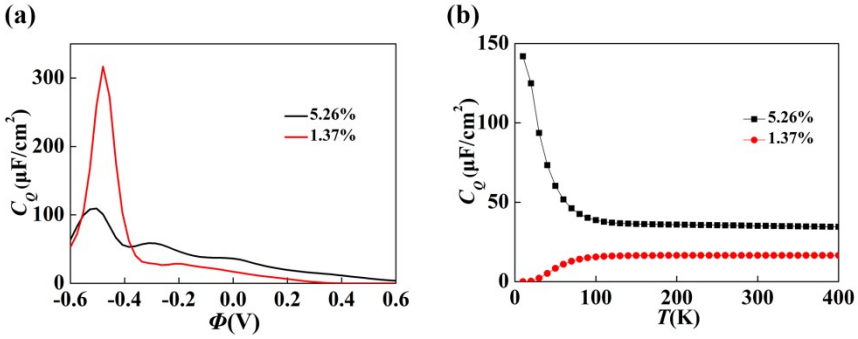

Fig. S7 C_Q of Cu adsorbed GDY with different concentrations as a function of (a) potential and (b) temperature.

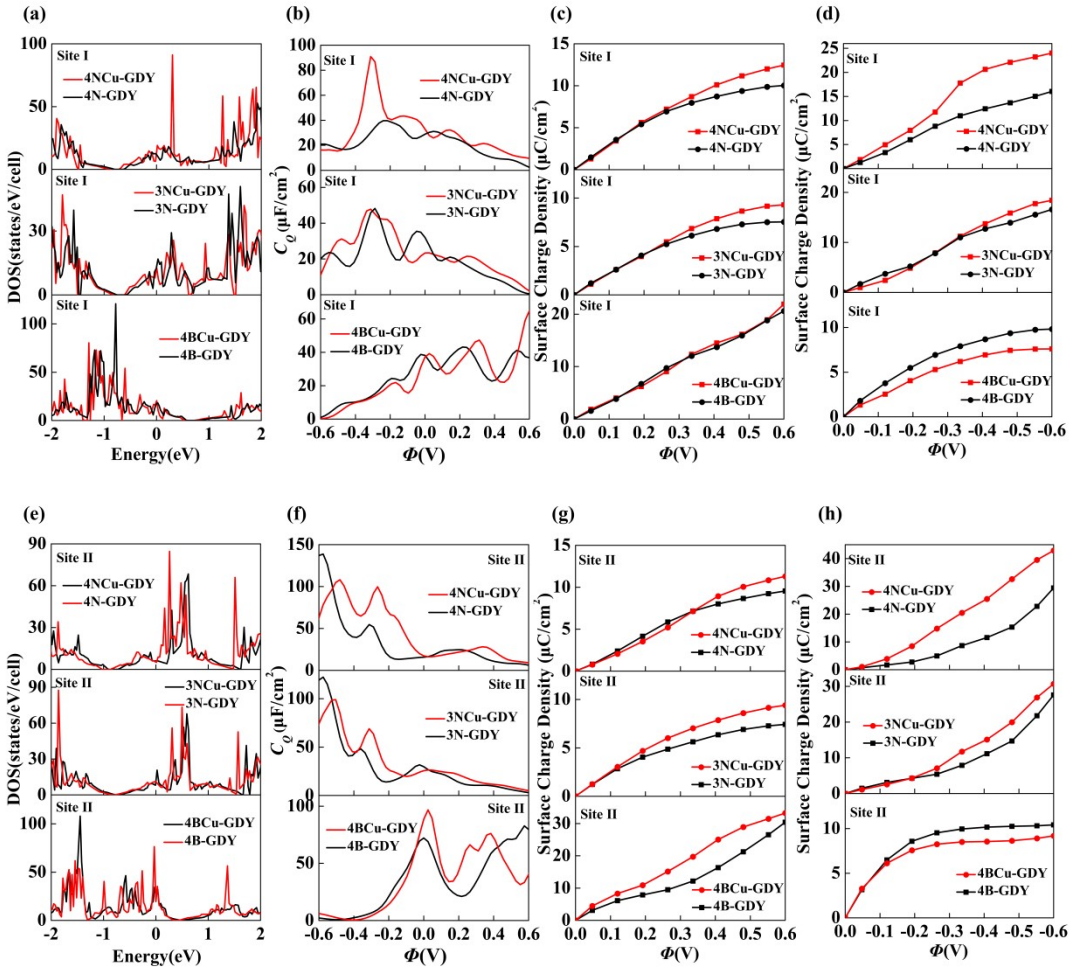

Fig. S8 Density of electronic states of 4BCu, 4NCu and 3NCu co-doped at I site (a) and II site (e); C_Q as a function of potential at I site (b) and II site (f), the potential range is -0.6~0.6V. Relationship between surface charge density and potential (-0.6~0.6V) at I site (c-d) and II site (g-h).

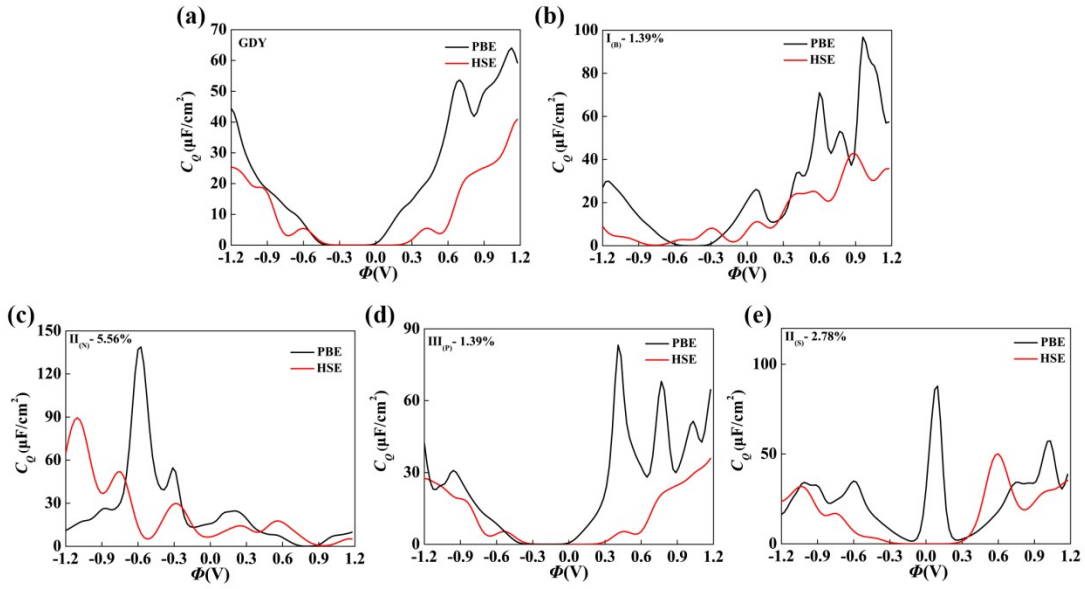

Fig. S9 Comparison of the C_Q of pristine and B/N/P/S-doped GDY calculated by HSE hybrid functional.

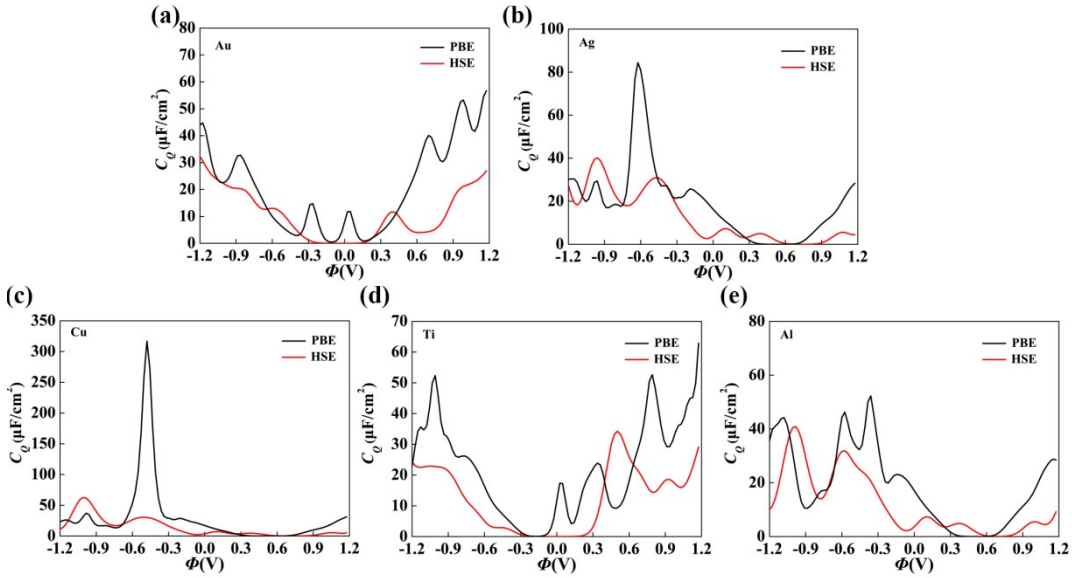

Fig. S10 Comparison of the C_Q of metal-adsorbed GDY calculated by HSE hybrid functional.

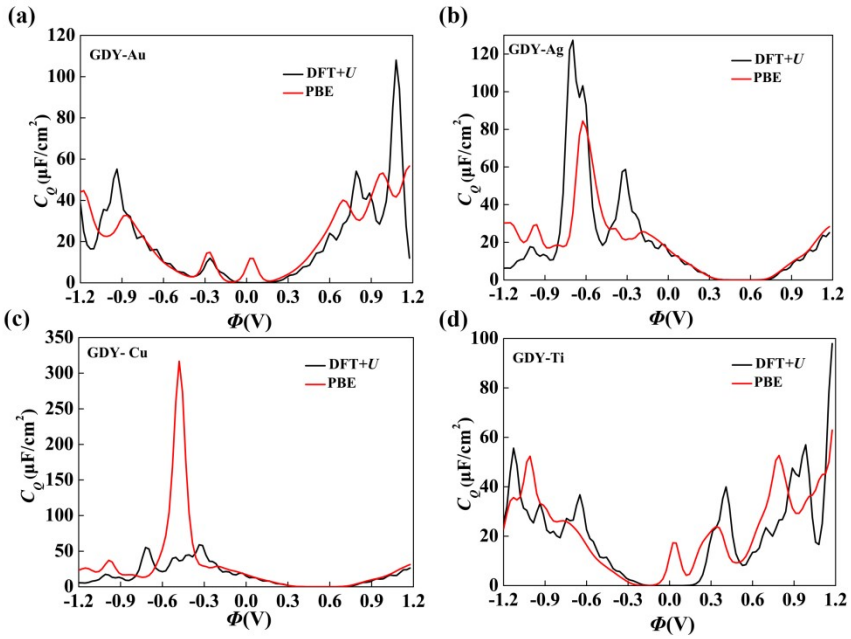

Fig. S11 Comparison of the C_Q of transition metal-adsorbed GDY after adding effective U value. The selected U value is 2.0 eV for Au[1], 2.0 eV for Ag[2], 2.5 eV for Ti[2], 6.52 eV for Cu[3] (Physical Review B, 2013, 87, 115111).

References

1. L. Avakyan, V. Durimanov, D. Nemesh, et al. *Opt. Mater.*, 2020, **109**, 110264.

2. M. I. Hussain, R. M. A. Khalil, F. Hussain, et al. *Mater. Res. Express*, 2020, **7**, 015906.

3. M. Heinemann, B. Eifert, C. Heiliger, *Phys. Rev. B*, 2013, **87**, 115111.