Supporting Information

Self-formed asymmetric Schottky contacts between graphene and $WSiGeN_4$

Dingbo Zhang[a,b], Fengai Zhao[b], Hongyan Wang[a,b], Yuxiang Ni[a,b] *

[a] Key Laboratory of Advanced Technologies of Materials, Ministry of Education of China, Southwest Jiaotong University, 610031 Chengdu, China

[b] School of Physical Science and Technology, Southwest Jiaotong University, 610031 Chengdu, China

Corresponding Author

* E-mail: yuxiang.ni@swjtu.edu.cn

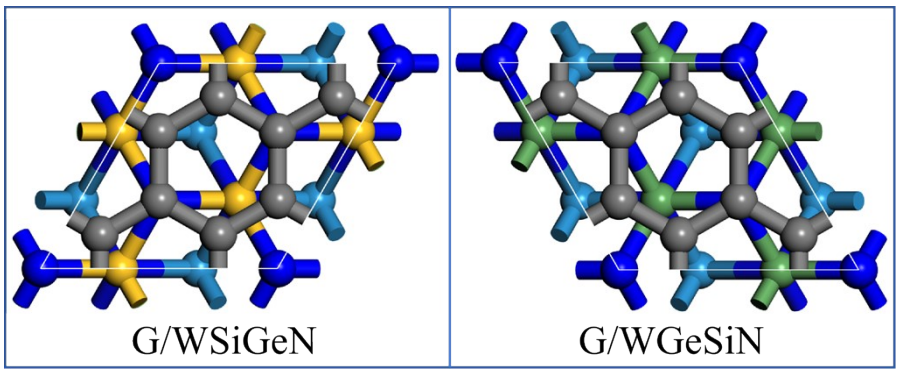

Figure S1. Top view of G/WSiGeN and G/WGeSiN heterostructures.

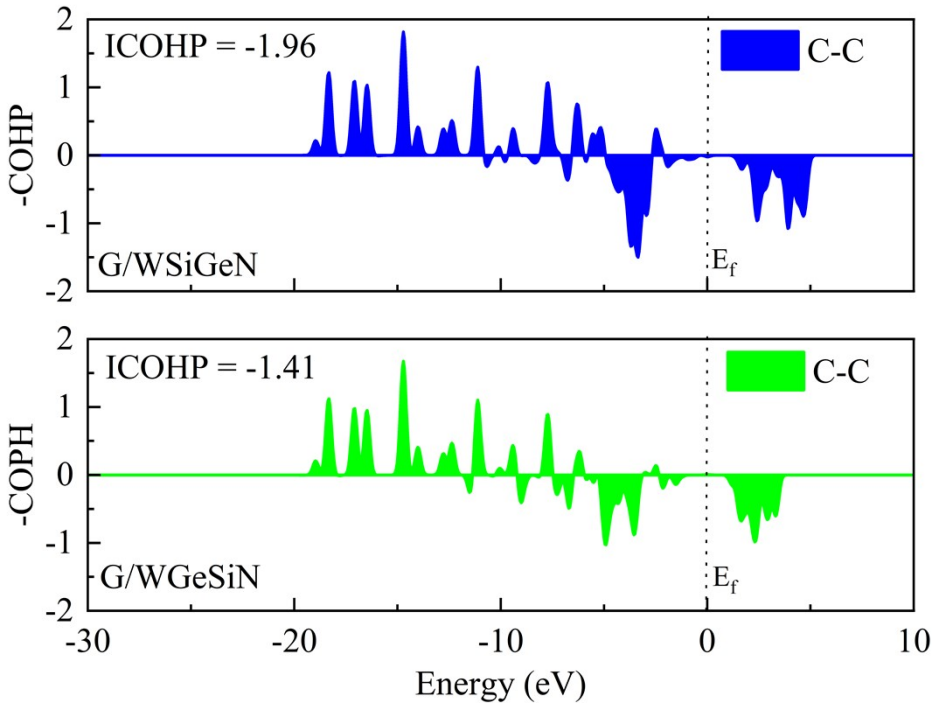

Figure S2. COHP between C atoms of G/WSiGeN and G/WGeSiN heterostructures.

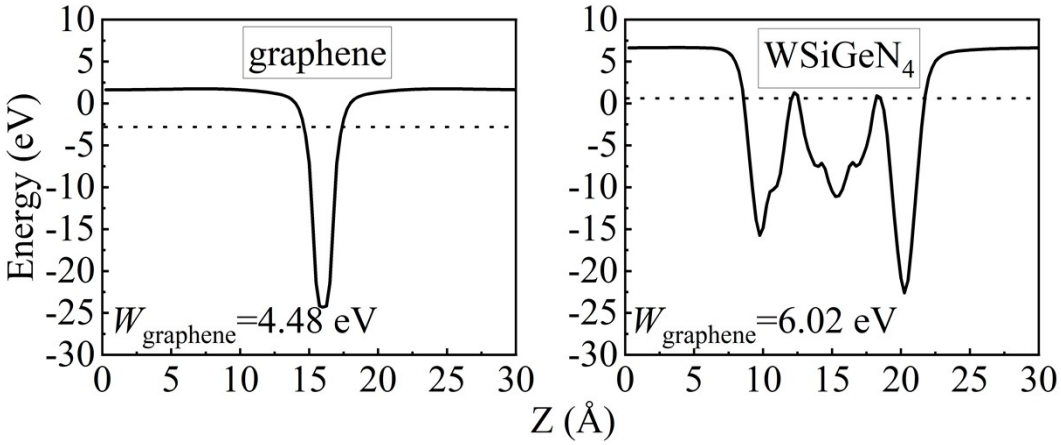

Figure S3. The electrostatic potentials and work functions of graphene and $WSiGeN_4$.

The work function The work function is defined as follows:

$$\Phi = E_{vac.} - E_F$$

where $E_{vac.}$ is the energy level of a stationary electron in the vacuum, E_F represents the Fermi level of the corresponding systems. Based on the formula, the work functions of graphene and $WSiGeN_4$ are 4.48 and 6.02 eV, respectively, as shown in Figure S3, implying that the electron transfer form graphene to $WSiGeN_4$.