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

SUPPLEMENTARY INFORMATION

First-principles study on Electronic and Optical Properties of the Type-II C_2N/g-ZnO van der Waals Heterostructure

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Phonon Spectrum Calculation

In order to verify the dynamical stability of C_2N/g-ZnO heterostructure, the phonon dispersion curves of C_2N/g-ZnO heterostructure were calculated. Due to the large system of the C_2N/g-ZnO heterostructure, we calculated the phonon band according to finite-differences method with a $2 \times 2 \times 1$ supercell including 128 atoms. It can be seen from the phonon band diagram that there is only tiny imaginary frequency near the G point as shown in Fig. S1, which may come from the acoustic nature. It will not affect the overall dynamical stability of heterostructure. It is proved that there is van der Waals force between layers of the heterostructure, and the heterostructure has a dynamical stability.

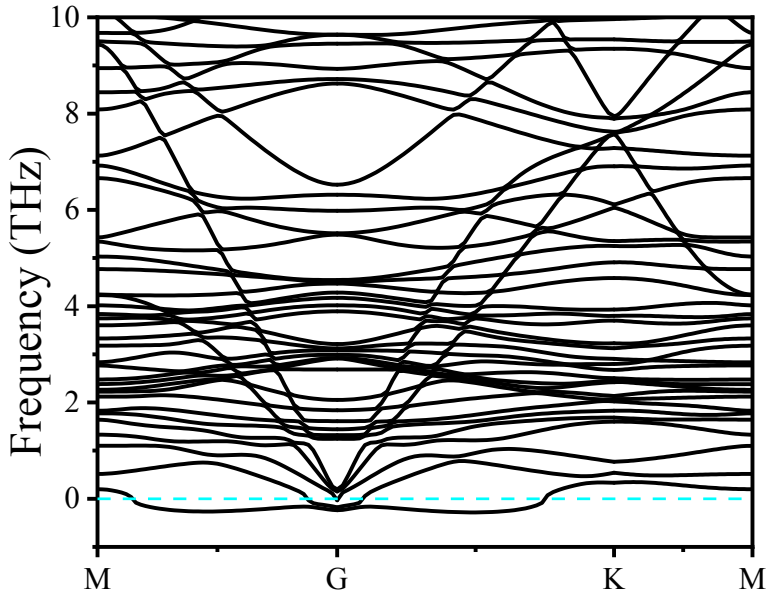

Figure S1. Phonon dispersion curves of C_2N/g-ZnO heterostructure

Ab Initio Molecular Dynamics Simulation

To further confirm the kinetic(thermal) stability of the C_2N/g-ZnO heterostructure, an ab initio molecular dynamics (AIMD) simulation is performed with a 2 × 2 × 1 supercell at 300 K and lasts 5 ps with a timestep of 1 fs. As shown in Fig. S2, both fluctuations of the total potential energy and the system temperature are very small, especially after 2 ps, indicating that the C_2N/g-ZnO heterostructure is thermally stable.

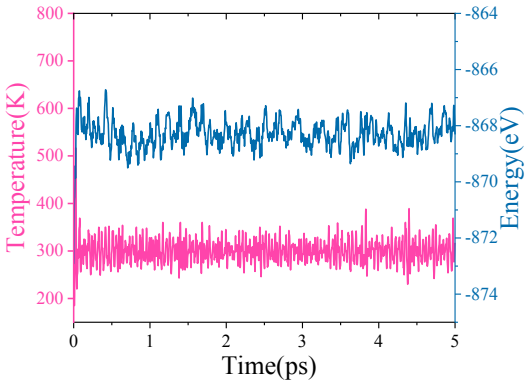

Figure S2. Variations of the total potential of the C_2N/g-ZnO heterostructure and the system temperature with simulation time.