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

Supporting Information

Stability of Hydrogen-terminated Graphene Edges

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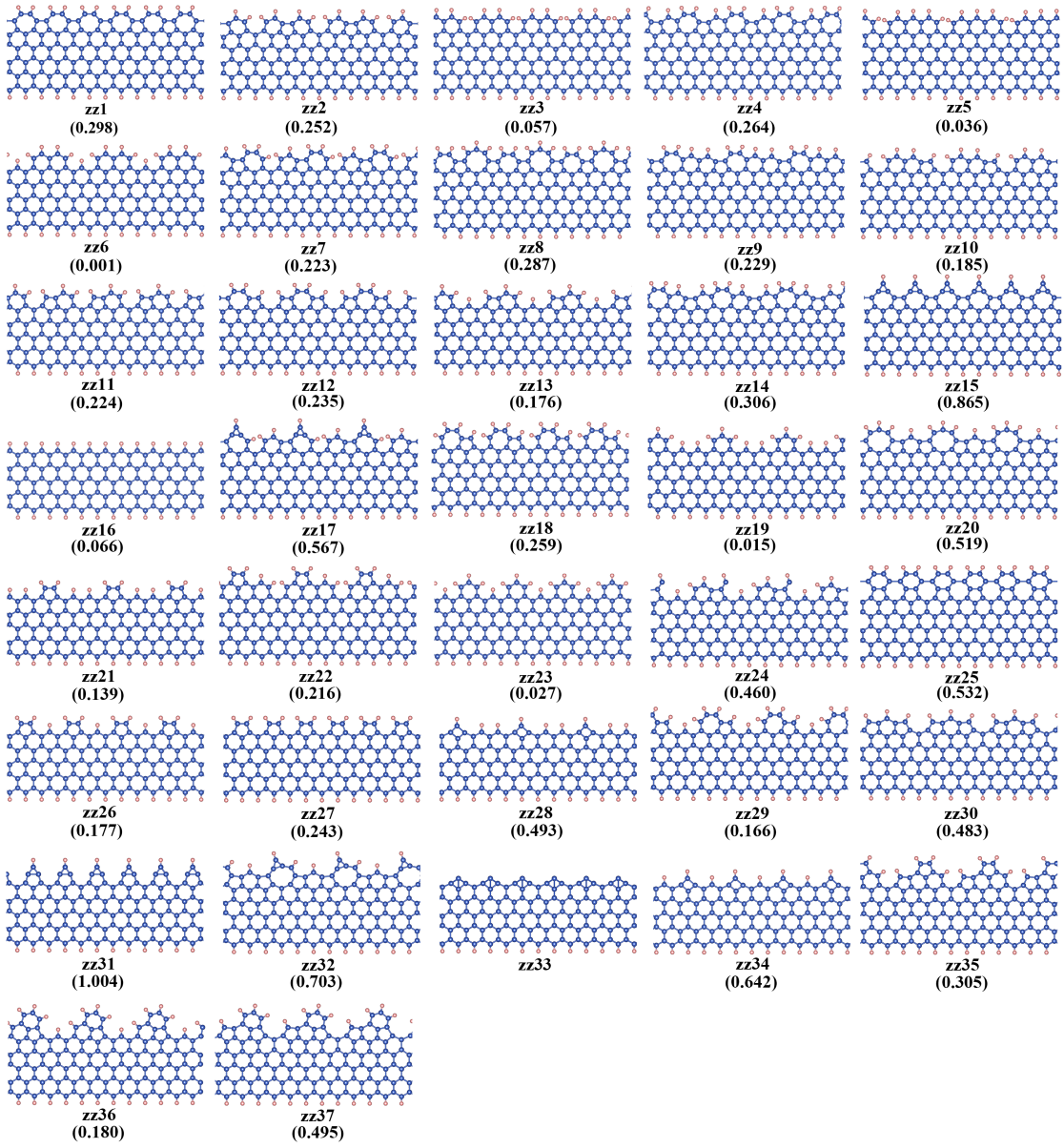
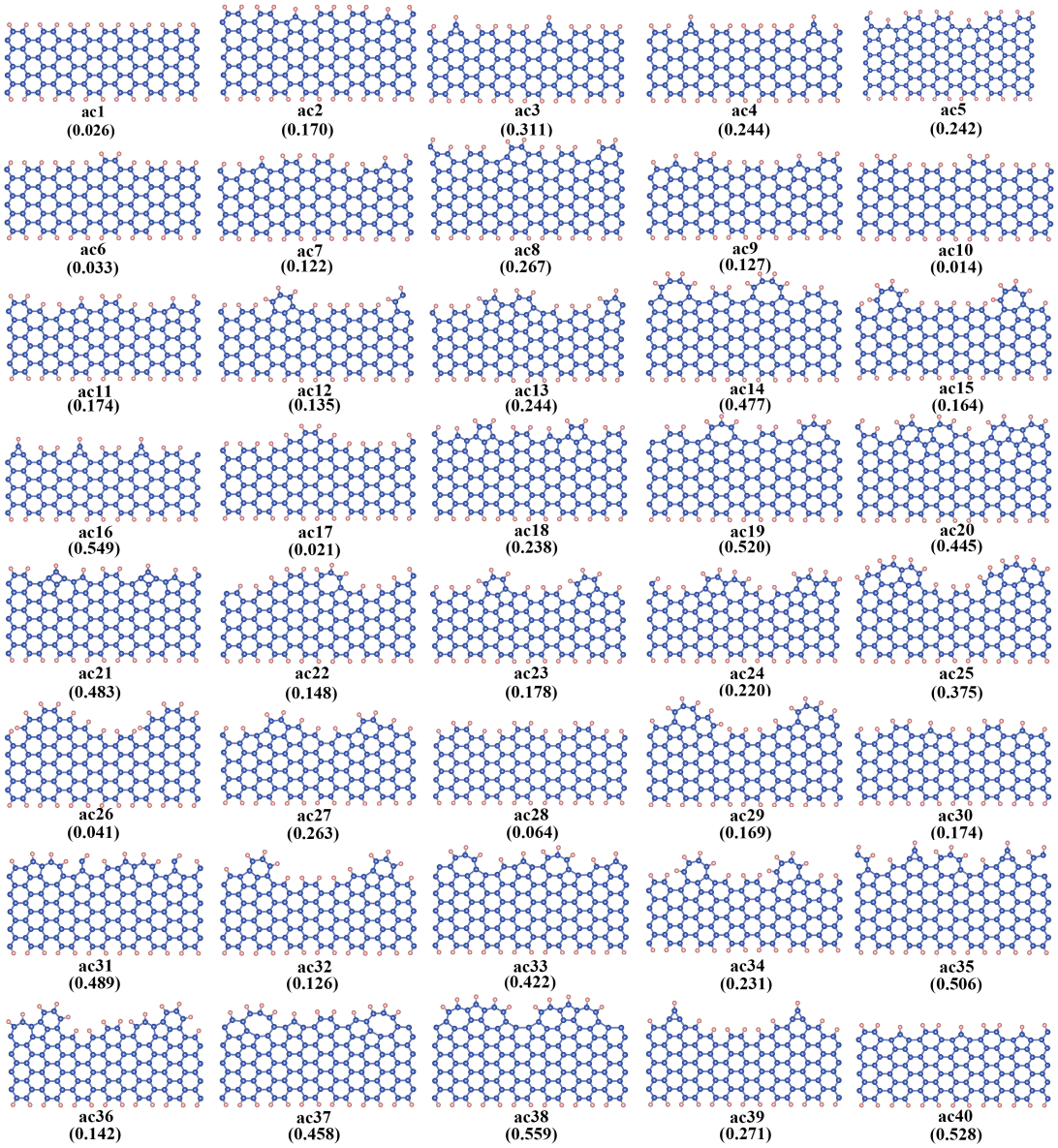
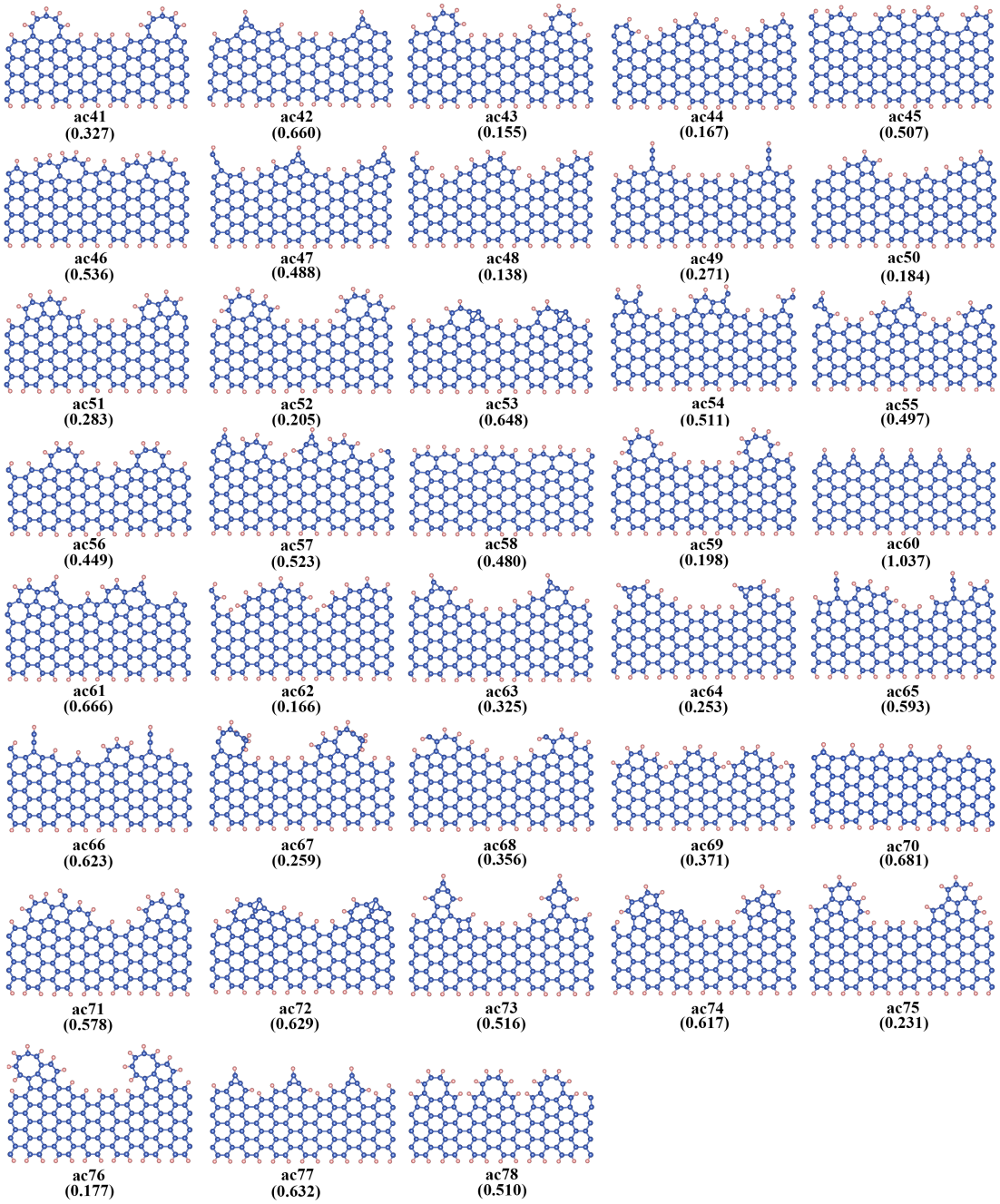


Fig S1. Configuration of the zigzag edges of graphene. The blue spheres represent C atoms and the pink spheres represent H atoms. The numbers in brackets represent the edge formation energy of corresponding H-termination structure. The unit of edge formation energy is (eV/Å).



(part 1)

Fig S2. Configuration of the armchair edges of graphene. The blue spheres represent C atoms and the pink spheres represent H atoms. The numbers in brackets represent the edge formation energy of corresponding H-termination structure. The unit of edge formation energy is (eV/Å).



(part 2)

Fig S2. Configuration of the armchair edges of graphene. The blue spheres represent C atoms and the pink spheres represent H atoms. The numbers in brackets represent the edge formation energy of corresponding H-termination structure. The unit of edge formation energy is (eV/Å).

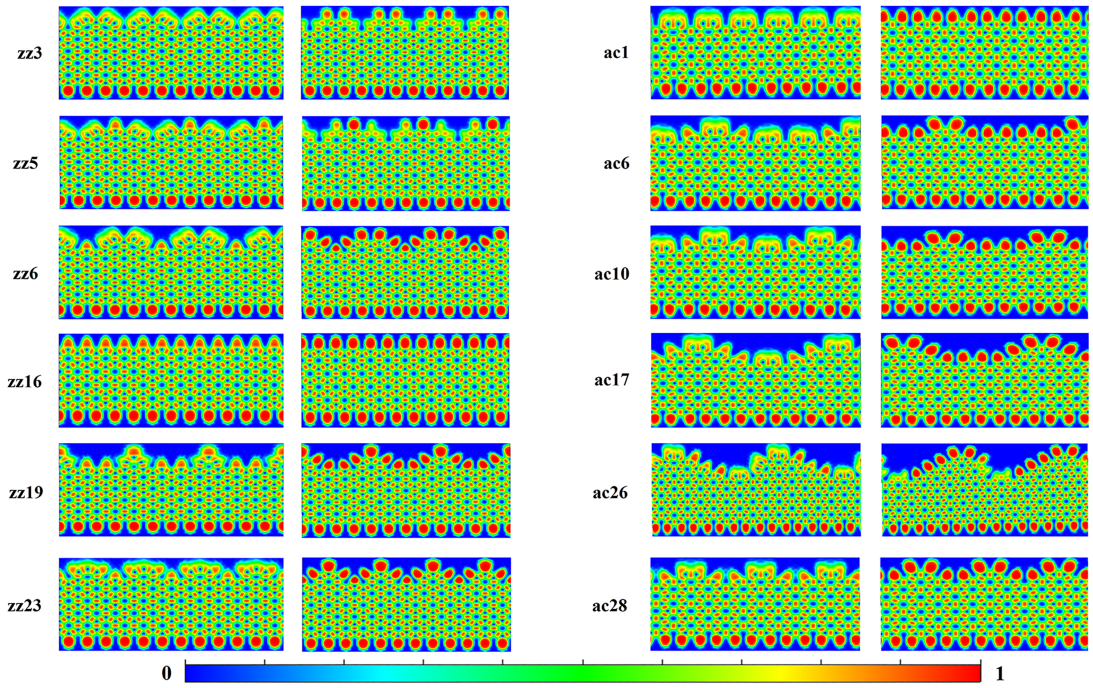


Fig S3. Electronic localization function (ELF) of six most stable zz-type and six most stable ac-type configurations. The left corresponds to the structures without H atom terminations, and the right corresponds to the structures with H atom terminations.

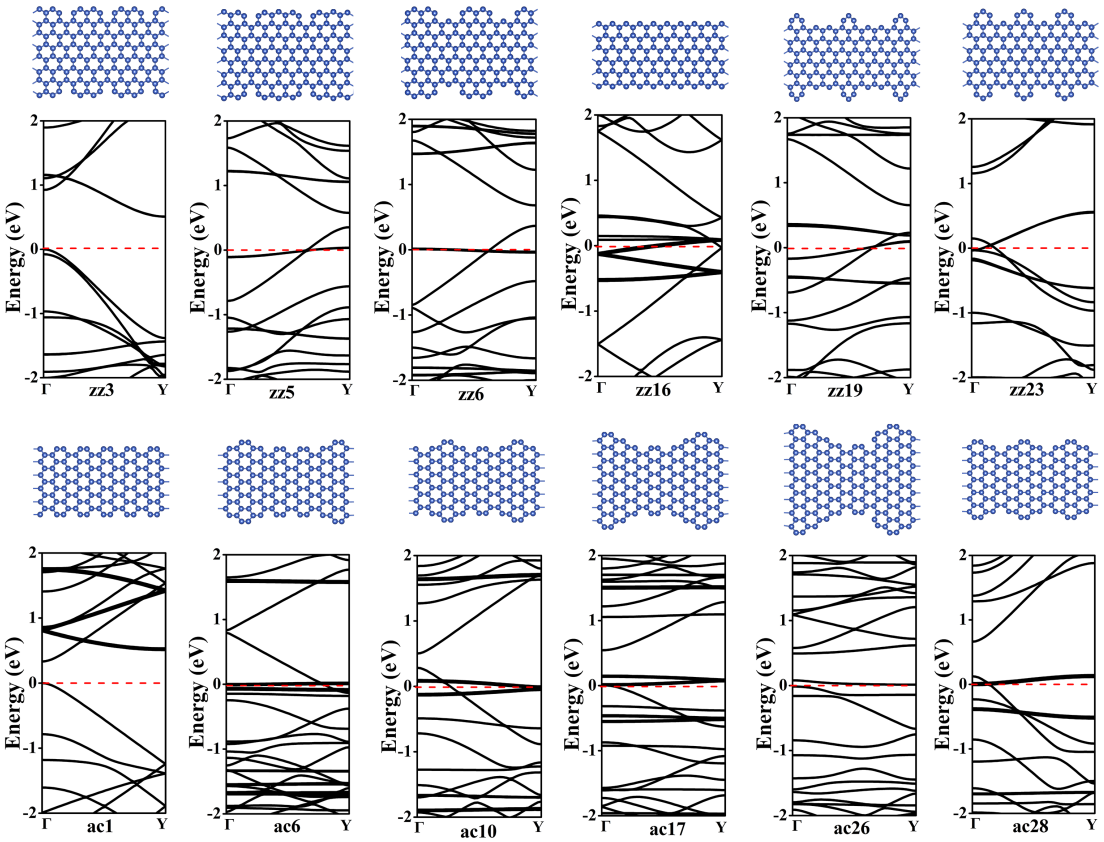


Fig S4. The band structures of six most stable zz-configurations and six most stable ac-configurations without H-termination.

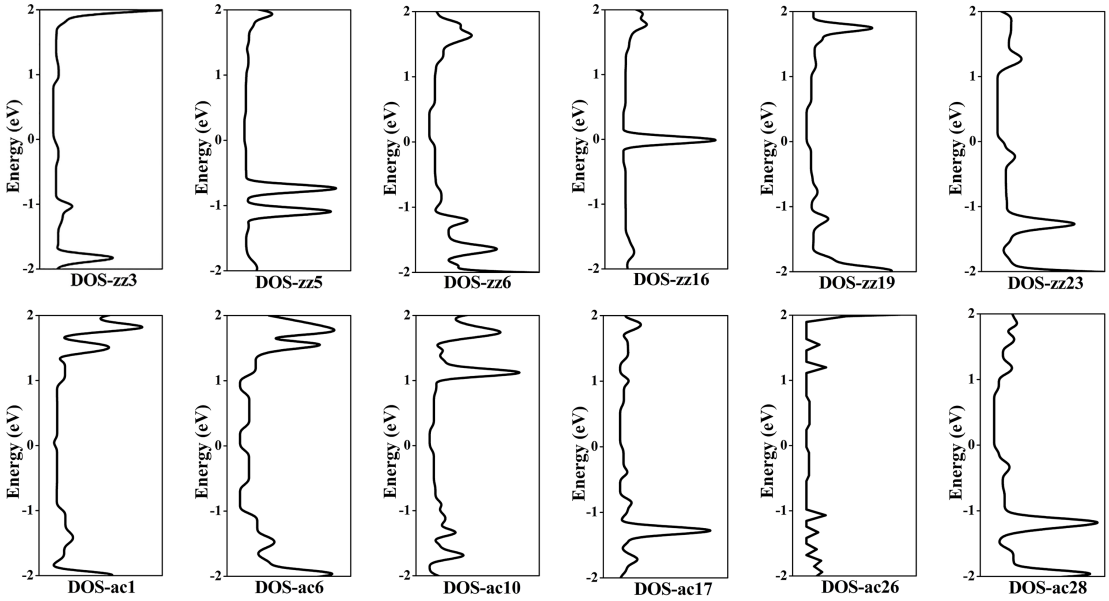


Fig S5. The density of state (DOS) of six most stable zz-configurations and six most stable ac-configurations with H-termination.