

Electronic Supplementary information

Spectral properties of B₄₀ enhanced by small molecule adsorption

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Part 1. The adsorption energy analysis

The formula for calculating adsorption energy as follows:

$$E_{\text{abs}} = E(\text{benzene-B}_{40}) - E(\text{B}_{40}) - E(\text{benzene}) - E(\text{BSSE})$$

Wherein, E_{abs} the adsorption energy, $E(\text{benzene-B}_{40})$ is the energy obtained from the optimized structures of benzene-B₄₀-6 and benzene-B₄₀-7, $E(\text{B}_{40})$ is the structural energy obtained from B₄₀ optimization, and $E(\text{benzene})$ is the structural energy obtained from the optimized structure of benzene, $E(\text{BSSE})$ refers to the basis set superposition error (BSSE) for the adsorption energy was corrected by implementing the counterpoise method.^{S1-S3} And the calculation results are $|E_{\text{abs}}(\text{benzene-B}_{40-6})| = 1.45$ eV, $|E_{\text{abs}}(\text{benzene-B}_{40-7})| = 1.44$ eV, thus the former is the more stable structure.

Part 2. The calculation details about structural optimization

All the computations are carried out using the Gaussian16 software package.²⁸ The convergence threshold of optimization are set to 4.5×10^{-4} Ha/Bohr for the Maximum Force, 3×10^{-4} Ha/Bohr for RMS Force, 1.8×10^{-3} Bohr for Maximum Displacement and 1.2×10^{-3} Bohr for RMS Displacement. For SCF, The density is converged to 10^{-8} .

Part 3. The analysis of electronic density difference

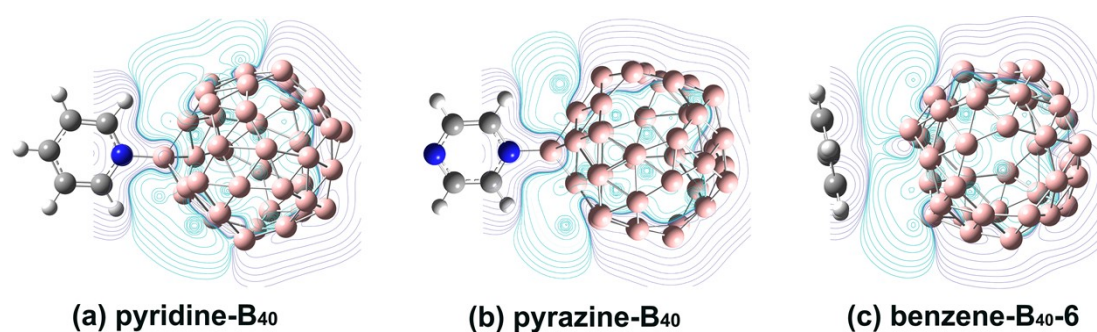


Figure S1 The analysis of electronic density difference. The purple and blue lines indicate electron accumulation and dissipation, respectively. Isovalue = 0.001 a.u..

References

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