

## Evaluation of the Adsorption Adaptability of Activated Carbon Using Dispersion Force

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**Abstract :** We attempted to predict adsorption coefficients by utilizing dispersion energies. We performed liquid-phase free energy calculations based on gas-phase geometries of organic compounds using the DFT and studied the relationship between the adsorption of organic compounds by activated carbon and dispersion energies of the organic compounds. A linear correlation between adsorption coefficients and dispersion energies was observed.

**Keywords :** activated carbon, adsorption, prediction, dispersion energy

**Conference Title :** ICCE 2016 : International Conference on Chemical Engineering

**Conference Location :** Singapore, Singapore

**Conference Dates :** November 21-22, 2016