

Accepted Manuscript

The influence of the functional group on activated carbon for acetone adsorption property by molecular simulation study

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PII: S1387-1811(17)30412-2

DOI: [10.1016/j.micromeso.2017.06.009](https://doi.org/10.1016/j.micromeso.2017.06.009)

Reference: MICMAT 8384

To appear in: *Microporous and Mesoporous Materials*

Received Date: 23 March 2017

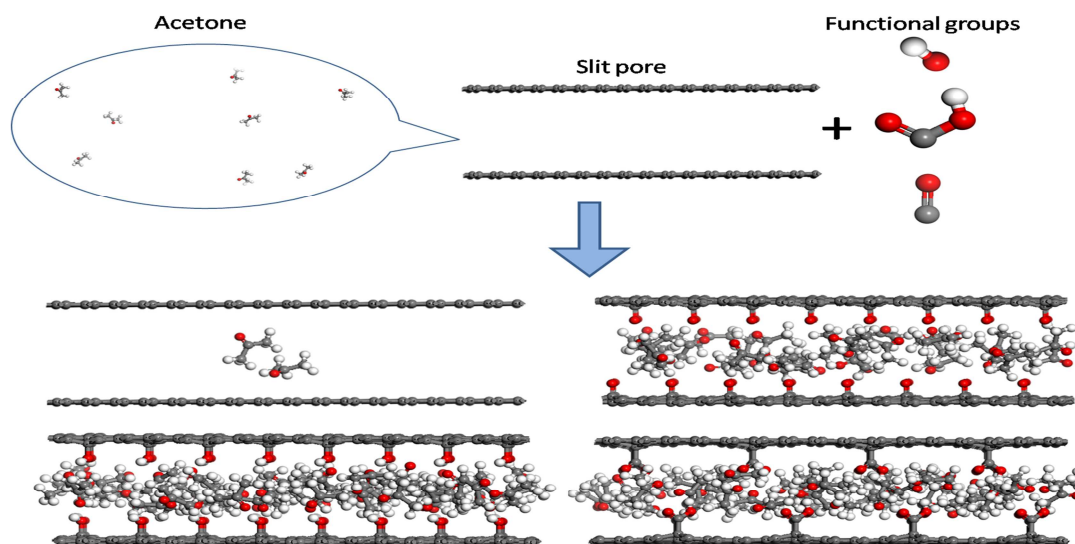
Revised Date: 9 May 2017

Accepted Date: 5 June 2017

Please cite this article as: X. Liang, J. Chi, Z. Yang, The influence of the functional group on activated carbon for acetone adsorption property by molecular simulation study, *Microporous and Mesoporous Materials* (2017), doi: 10.1016/j.micromeso.2017.06.009.

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Graphical Abstract



1) Trace acetone in indoor air (10ppmv) is mainly adsorbed in graphitic pore with 1.0nm pore width. 2) Functional groups especially carboxyl or hydroxyl in micro pores, which has electrostatic interactions with acetone molecule, greatly increase adsorption amount of trace acetone (10ppm). 3) Adsorption amount of acetone in pores is determined by isosteric heat and available adsorption sites on pore wall.

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