

DFT Model Number	DFT Model Description
mod000.df2	N2@77-Carbon, Slit pores, Original DFT
mod001.df2	Ar@87-Carbon, Slit pores, Original DFT
mod003.df2	N2 - Modified Density Functional
mod004.df2	N2 @ 77K, Slit Pore, Halsey Thickness Curve
mod005.df2	N2 @ 77K, Cylinder Pore, Halsey Thickness Curve
mod006.df2	N2 @ 77K, Slit Pore, Harkins and Jura Model
mod007.df2	N2 @ 77K, Cylinder Pore, Harkins and Jura Model
mod008.df2	N2 @ 77K, Slit Pore, Broekhoff – de Boer Model
mod009.df2	N2 @ 77K, Cylinder Pore, Broekhoff – de Boer Model
mod010.df2	N2@77-Oxide Cyl Pores, Strong Potential
mod011.df2	CO2 @ 273 on Carbon, Slit Pores
mod012.df2	AR - Modified Density Functional
mod013.df2	N2@77-Oxide Cylindrical Pores,Tarazona
mod014.df2	N2@77 Cyl Pores in Pillared Clay, NLDFT
mod015.df2	Ar@87 in Oxide Cyl Pores, NLDFT
mod023.df2	Ar@77 on Carbon Slit Pores by NLDFT
mod024.df2	N2@87 on Carbon Slit Pores by NLDFT
mod101.df2	Argon on Carbon at 77 Kelvin, slit like pores
mod102.df2	Ar@77 on Zeolite Cyl Pores, NLDFT
mod110.df2	2D-NLDFT, N2-Carbon Finite Pores, As=6
mod111.df2	2D-NLDFT, N2-Carbon Finite Pores, Aspect=4
mod112.df2	NLDFT(SD3), N2-77-Carbon Slit Pores
mod200.df2	N2 @ 77 on Carbon Slit Pores
mod200.df3	N2 @ 77 on Carbon Slit Pores by NLDFT
mod201.df2	N2@77-Carb Finite Pores, As=4, 2D-NLDFT
mod202.df2	N2@77-Carb Finite Pores, As=6, 2D-NLDFT
mod203.df2	Ar@87 on Carbon Slit Pores by NLDFT
mod204.df2	Ar@87-Carb Finite Pores, As=4, 2D-NLDFT
mod205.df2	Ar@87-Carb Finite Pores, As=6, 2D-NLDFT
mod206.df2	N2@77-Carb Finite Pores, As12, 2D-NLDFT
mod207.df2	Ar@87-Carb Finite Pores,As=12, 2D-NLDFT
mod225.df2	N2@77-Carb Cyl Pores, SWNT, NLDFT
mod226.df2	N2@77-Carb Cyl Pores, MWNT, NLDFT
mod227.df2	Ar@87-Carb Cyl Pores, SWNT, NLDFT
mod228.df2	Ar@87-Carb Cyl Pores, MWNT, NLDFT
mod229.df2	Ar@77-Zeolites, H-Form, NLDFT
mod230.df2	Ar@77-Zeolites, Me-Form, NLDFT
mod241.df2	GCMC CO2 Carbon slit
mod250.df2	CO2@273-Carbon Slit Pores, 10 atm,NLDFT
mod251.df2	Ar@87-Zeolites, H-Form, NLDFT
mod252.df2	Ar@87-Zeolites, Me-Form, NLDFT
mod255.df2	HS-2D-NLDFT, Carbon, N2, 77

mod300.df2	NLDFT, Ultramicroporous Zeolites, O2, 77
mod300.df3	NLDFT, Ultramicroporous Zeolites, O2, 77
mod310.df2	NLDFT, Ultramicroporous Zeolites, H2, 77
mod310.df3	NLDFT, Ultramicroporous Zeolites, H2, 77
mod400.df3	CO2@273-Carbon, NLDFT
mod410.df2	HS-2D-NLDFT, Carbon, O2, 77
mod420.df2	HS-2D-NLDFT, Carbon, Ar, 87
mod425.df2	HS-2D-NLDFT, Carbon, CO2, 273
mod430.df2	HS-2D-NLDFT, Carbon, H2, 77
mod440.df2	HS-2D-NLDFT, Carb Cyl Pores (ZTC) N2@77
mod450.df2	HS-2D-NLDFT, Carb Cyl Mesopores, N2@77
mod600.df2	MOF1-Ar Cylindrical Mesopores, 2D-NLDFT
mod610.df2	HS-2D-NLDFT, Cylindrical Oxide, Ar, 87

Model References

1. P. Tarazona. **Free-energy density functional for hard spheres**. Phys. Rev. A, 31(4):2672–2679, Apr 1985.
2. P. Tarazona, U. Marini Bettolo Marconi, and R. Evans. **Phase equilibria of fluid interfaces and confined fluids – non-local versus local density functionals**. Molecular Physics: An International Journal at the Interface Between Chemistry and Physics, 60(3):573–595, 1987.
3. Christian Lastoskie, Keith E. Gubbins, and Nicholas Quirke. **Pore size distribution analysis of microporous carbons: a density functional theory approach**. The Journal of Physical Chemistry, 97(18):4786–4796, May 1993.
4. P. Tarazona. **A density functional theory of melting**. Molecular Physics: An International Journal at the Interface Between Chemistry and Physics, 52(1):81–96, 1984.
5. James P. Olivier. **Modeling physical adsorption on porous and nonporous solids using density functional theory**. Journal of Porous Materials, 2(1):9–17, July 1995.
6. James P. Olivier. Improving the models used for calculating the size distribution of micropore volume of activated carbons from adsorption data. Carbon, 36(10):1469–1472, October 1998.
7. M. W. Maddox, J. P. Olivier, and K. E. Gubbins. **Characterization of mcm-41 using molecular simulation: Heterogeneity effects**. Langmuir, 13(6):1737–1745, Mar 1997.
8. M. Jaroniec, M. Kruk, J.P. Olivier, and S. Koch. **A new method for the accurate pore size analysis of mcm -41 and other silica based mesoporous materials**. In Unger K.K., Kreysa G., and J. P. Baselt, editors, Proceedings of the Fifth International Symposium on the Characterization of Porous Solids, COPS-V, volume 128 of Studies in Surface Science and Catalysis, page 71. Elsevier, 2000.
9. James P. Olivier and Mario L. Occelli. **Surface area and microporosity of a pillared interlayered clay (pilc) from a hybrid density functional theory (dft) method**. The Journal of Physical Chemistry B, 105(22):5358–5358, May 2001.

10. M. L. Occelli, J. P. Olivier, J. A. Perdigon-Melon, and A. Auroux. **Surface area, pore volume distribution, and acidity in mesoporous expanded clay catalysts from hybrid density functional theory (dft) and adsorption microcalorimetry methods**. Langmuir, 18(25):9816–9823, Nov 2002.
11. Mario L. Occelli, James P. Olivier, Alice Petre, and Aline Auroux. Determination of pore size distribution, **surface area, and acidity in fluid cracking catalysts (fccs) from nonlocal density functional theoretical models of adsorption and from microcalorimetry methods**. The Journal of Physical Chemistry B, 107(17):4128–4136, Apr 2003.
12. M. L. Occelli, J. P. Olivier, A. Auroux, M. Kalwei, and H. Eckert. **Basicity and porosity of a calcined hydrotalcite-type material from nitrogen porosimetry and adsorption microcalorimetry methods**. Chemistry of Materials, 15(22):4231–4238, Oct 2003.
13. Jacek Jagiello and James P. Olivier. **A simple two-dimensional NLDFT model of gas adsorption in finite carbon pores. Application to pore structure analysis**. The Journal of Physical Chemistry C, 113(45):19382–19385, Oct 2009.
14. J. Jagiello and J. P. Olivier, **2D-NLDFT Adsorption Models for Carbon Slit-Shaped Pores with Surface Energetical Heterogeneity and Geometrical Corrugation**. Carbon (2013) 55, 70-80.
15. J. Jagiello, J. Kenvin, J. Olivier, A. Lupini, C. Contescu, **Using a new finite slit pore model for NLDFT analysis of carbon pore structure**, Adsorption Science & Technology 29 (2011) 769-780.
16. J. Jagiello, J.P. Olivier, **Carbon slit pore model incorporating surface energetical heterogeneity and geometrical corrugation**, Adsorption 19 (2013) 777-783
17. J. Jagiello, J. Kenvin, **Consistency of Carbon Nanopore Characteristics Derived from Adsorption of Simple Gases and 2D-NLDFT Models. Advantages of Using Adsorption Isotherms of Oxygen (O₂) at 77 K**, Journal of Colloid and Interface Science 542 (2019) 151-158.
18. J. Jagiello, C. Ania, J.B. Parra, C. Cook, **Dual gas analysis of microporous carbons using 2D-NLDFT heterogeneous surface model and combined adsorption data of N₂ and CO₂**, Carbon 91 (2015) 330-337.
19. J. Jagiello, J. Kenvin, C.O. Ania, J.B. Parra, A. Celzard, V. Fierro, **Exploiting the adsorption of simple gases O₂ and H₂ with minimal quadrupole moments for the dual gas characterization of nanoporous carbons using 2D-NLDFT models**, Carbon 160 (2020) 164-175.
20. J. Jagiello, J. Kenvin, A. Celzard, V. Fierro, **Enhanced resolution of ultra micropore size determination of biochars and activated carbons by dual gas analysis using N₂ and CO₂ with 2D-NLDFT adsorption models**, Carbon 144 (2019) 206-215.
21. J. Jagiello, T. Kyotani, H. Nishihara, **Development of a simple NLDFT model for the analysis of adsorption isotherms on zeolite templated carbon (ZTC)**, Carbon 169 (2020) 205-213.
22. P. Li, Q. Chen, T.C. Wang, N.A. Vermeulen, B.L. Mehdi, A. Dohnalkova, N.D. Browning, D. Shen, R. Anderson, D.A. Gómez-Gualdrón, F.M. Cetin, J. Jagiello, A.M. Asiri, J.F. Stoddart, O.K. Farha, **Hierarchically Engineered Mesoporous Metal-Organic Frameworks toward Cell-free Immobilized Enzyme Systems**, Chem (2018) 4, 1022-1034.
23. J. Jagiello, M. Jaroniec, **2D-NLDFT Adsorption Models for Porous Oxides with Corrugated Cylindrical Pores**, Journal of Colloid and Interface Science 532 (2018) 588-597.