[1] 范荣香. 中国炼焦煤资源与煤焦化产业发展分析[J]. 化学工业, 2008, 26(5):1-8.

[2] 马庆元. 中国炼焦煤资源的分布特征[J]. 煤炭科学技术, 2004, 32(3):63-66.

[3] 王胜春, 张德祥, 陆鑫,等. 中国炼焦煤资源与焦炭质量的现状与展望[J]. 煤炭转化, 2011, 34(3):92-96.

[4] 毛德荣, 侯振才. 全国煤炭资源开发利用现状与保护对策的探讨[J]. 中国地质, 1997(1):14-17.

[5] 杜铭华. 中国炼焦煤资源及生产[J]. 煤质技术, 2006(6):1-3.

[6] 张崇欣, 宋奇文, 马剑. 基于AHP的中国煤炭资源开发利用现状分析[J]. 煤矿现代化, 2010(5):5-6.

[7] 宋冬林, 赵震宇. 中国煤炭资源利用现状及成因分析——基于不可再生资源经济学的视角[J]. 求是学刊, 2009, 36(5).

[8] 曹代勇, 黄岑丽, 袁文峰,等. 山西炼焦煤资源与开发利用现状分析[J]. 中国煤炭地质, 2008, 20(11):1-4.

[9] 黄文辉, 杨起, 唐修义,等. 中国炼焦煤资源分布特点与深部资源潜力分析[J]. 中国煤炭地质, 2010, 22(5):1-6.

[10] 王传格, 张妮, 陈燕. 煤显微组分结构特征及其与热解行为的关系[J]. 煤炭转化, 2011, 34(3):11-16.

[11] Peng Xia, Kunjie Li\*, Fangui Zeng\*, Xiong Xiao, Jianliang Zhang, Jianhua Xiang, Beilei Sun. Pyrolysis characteristic of coals with different metamorphic grades and its instruction to coalbed methane development. World Journal of Engineering, 2017, 14(5): 423-432.

[12] Fuchs W . Thermodynamic treatment of the swelling pressure of coal[J]. Journal of the Franklin Institute, 1941, 231(2):103-119.

[13] 李霞, 曾凡桂, 王威, et al. 低中煤级煤结构演化的FTIR表征[J]. 煤炭学报, 2015, 40(12):2900-2908.

[14] 罗陨飞, 李文华, 陈亚飞. 中低变质程度煤显微组分结构的~(13)C-NMR研究[J]. 燃料化学学报, 2005, 33(5):540-543.

[15] Given P H , Cronauer D C , Spackman W , et al. Dependence of coal liquefaction behaviour on coal characteristics. 2. Role of petrographic composition[J]. Fuel, 1975, 54(1):40-49.

[16] Given P H. An Essay on the Organic Geochemistry of Coal[J]. Coal Science, 1984:63-252.

[17] Wiser W H, Hill G R, Kertamus N J. Kinetic Study of Pyrolysis of High Volatile Bituminous Coal[J]. Industrial & Engineering Chemistry Process Design & Development, 1967, 10:2(1):133-138.

[18] Chemistry and catalysis of coal liquefaction: catalytic and thermal upgrading of coal liquids: and hydrogenation of CO to produce fuels. Volume V. Final report. [5,6-benzoquinoline, 7,8-benzoquinoline, phenanthridine][J]. 1985.

[19] Shinn J H. From coal to single-stage and two-stage products: A reactive model of coal structure[J]. Fuel, 1984, 63(9):1187-1196.

[20] FAULON, J.L, HATCHER, et al. A computer-aided molecular model for high volatile bituminous coal[J]. Fuel Processing Technology, 1993, 34(3):277-293.

[21] FAULON, J. L, VANDENBROUCKE, et al. 3D Chemical model for geological macromolecules[J]. Organic Geochemistry, 1990, 16(4):981-993.

[22] Brown J K, Hirsch P B. Recent Infra-Red and X-Ray Studies of Coal[J]. Nature, 1955, 175(4449):229-233.

[23] Cartz L, Diamond R, Hirsch P B. New X-Ray Data on Coals[J]. Nature, 1956, 177(4507):500-502.

[24] Hirsch P B. X-Ray Scattering from Coals[J]. Proceedings of the Royal Society A, 1954, 226(1165):143-169.

[25] Cartz L, Hirsch P B. A Contribution to the Structure of Coals from X-Ray Diffraction Studies[J]. Philosophical Transactions of the Royal Society of London, 1960, 252(1019):557-602.

[26] Miller R N, Given P H. The association of major, minor and trace inorganic elements with lignites. I. Experimental approach and study of a North Dakota lignite[J]. Geochimica Et Cosmochimica Acta, 1986, 50(9):2033-2043.

[27] Miller R N, Given P H. The association of major, minor and trace inorganic elements with lignites. I. Experimental approach and study of a North Dakota lignite[J]. Geochimica Et Cosmochimica Acta, 1986, 50(9):2033-2043.

[28] Nishioka M. The associated molecular nature of bituminous coal[J]. Fuel, 1992, 71(8):941-948.

[29] Nishioka M, Campbell R M, Lee M L, et al. Isolation of sulphur heterocycles from petroleum- and coal-derived materials by ligand exchange chromatography[J]. Fuel, 1986, 65(2):270-273.

[30] Nishioka M, Lee M L, Castle R N. Sulphur heterocycles in coal-derived products : Relation between structure and abundance[J]. Fuel, 1986, 65(3):390-396.

[31] Lafdi K, Bonnamy S, Oberlin A. Tem studies of coal tars: Crude tar and its insoluble fractions[J]. Carbon, 1990, 28(1):57-63.

[32] Lafdi K, Bonnamy S, Oberlin A. TEM studies of coal tars effects of stresses (filtration and decantation)[J]. Carbon, 1990, 28(5):617-629.

[33] LAFDI, BONNAMY, OBERLIN. Tem studies of coal tars influence of distillation process at increasing temperature[J]. Carbon, 1990, 28(5):631-640.

[34] Grigoriew H. Diffraction studies of coal structure ☆[J]. Fuel, 1990, 69(7):840-845.

[35] Grigoriew H, Cichowska G. Spatial coal structure models[J]. Journal of Applied Crystallography, 2010, 23(3):209-210.

[36] 曲星武, 王金城. 煤的X射线分析[J]. 煤田地质与勘探, 1980(2):36-43.

[37] 贾建波, 曾凡桂, 孙蓓蕾. 神东2-2煤镜质组大分子结构模型13C-NMR谱的构建与修正[J]. 燃料化学学报, 2011, 39(9).

[38] Xiang J H, Zeng F G, Liang H Z, et al. Model construction of the macromolecular structure of Yanzhou coal and its molecular simulation[J]. Journal of Fuel Chemistry & Technology, 2011, 39(7):481-488.

[39] Xiang J H, Zeng F G, et al. Construction of macromolecular structural model of anthracite from Chengzhuang coal mine and its molecular simulation[J]. Journal of Fuel Chemistry & Technology, 2013, 41(4):391-400.

[40] 马延平, 相建华, 李美芬, et al. 柳林3#镜煤吡啶残煤大分子结构模型及分子模拟[J]. 燃料化学学报, 2012, 40(11).

[41] 张莉, 曾凡桂, 相建华. 内蒙五牧场矿区11号煤层原煤大分子结构特征及其形成机制[J]. 燃料化学学报, 2013, 41(11):1294-1302.

[42] Mathews J P , Chaffee A L . The molecular representations of coal – A review[J]. Fuel, 2012, 96(none):1-14.

[43] 司加康, 马兰8号煤大分子结构模型构建及分子模拟[D]. 太原理工大学, 2014.

[44] 姜永泼, 屯兰2号镜煤大分子聚集态结构模型的构建及分子模拟[D]. 2018.

[45] Crone B, Dodabalapur A, Gelperin A, et al. Electronic sensing of vapors with organic transistors[J]. Applied Physics Letters, 2001, 78(15):2229.

[46] Gershenson M E, Podzorov V, Morpurgo A F. Colloquium: Electronic transport in single-crystal organic transistors[J]. Review of Modern Physics, 2006, 78(3):973-989.

[47] Tan C M, ROY, Arijit. Electromigration in ULSI interconnects[J]. Materials Science & Engineering R, 2007, 58(1):1-75.

[48] Nickolls J, Dally W J. The GPU Computing Era[J]. IEEE Micro, 2010, 30(2):56-69.

[48] Hogerheijde M R, Van d T F F S. An accelerated Monte Carlo method to solve two-dimensional radiative transfer and molecular excitation[J]. Astronomy & Astrophysics, 2000, 362(2000):697-710.

[49] Surendra K. Jain,†, Roland J.M. Pellenq,‡, Jorge P. Pikunic,§ and, et al. Molecular Modeling of Porous Carbons Using the Hybrid Reverse Monte Carlo Method[J]. Langmuir the Acs Journal of Surfaces & Colloids, 2006, 22(24):9942-8.

[50] Chen J, Fang Q, Intes X. Mesh-based Monte Carlo method in time-domain widefield fluorescence molecular tomography[J]. Journal of Biomedical Optics, 2012, 17(10):106009.

[51] Rozenberg L A M J. Quantum Monte Carlo method for models of molecular nanodevices[J]. Physical Review B, 2005, 72(4):1301.

[52] Bhushan B. Molecular Dynamics Method[M]// Encyclopedia of Nanotechnology. 2012.

[53] Parrinello M. Polymorphic transitions in single crystals: A new molecular dynamics method[J]. Journal of Applied Physics, 1981, 52(12):7182-7190.

[54] Nosé S. A molecular dynamics method for simulations in the canonical ensemble[J]. Molecular Physics, 2002, 100(1):191-198.

[55] Carlson G A. Computer simulation of the molecular structure of bituminous coal[J]. Energy & Fuels, 1992, 6(6):771-778.

[56] Provine W D , Klein M T . Molecular simulation of thermal direct coal liquefaction[J]. Chemical Engineering Science, 1994, 49(24-part-PA):4223-4248.

[57] Honggang C , Fan L , Kechang X . STUDY ON CAMD FOR COAL STRUCTURE[J]. COAL CONVERSION, 1996.

[58] Takanohashi T , Iino M , Nakamura K . Simulation of Interaction of Coal Associates with Solvents Using the Molecular Dynamics Calculation[J]. Energy & Fuels, 1998, 12(6):1168-1173.

[59] Ma X, Dong X, Fan Y. Prediction and Characterization of the Microcrystal Structures of Coal with Molecular Simulation[J]. Energy & Fuels, 2018:acs.energyfuels.7b03698.

[60] 闫金定, 崔洪, 杨建丽,等. 热重质谱联用(TG/MS)技术应用进展[J]. 分析测试学报, 2003, 22(4):104-107.

[61] 李淑娥, 王晓东, 颜国纲,等. 热重-质谱联用技术(TG-MS)及系统优化研究[J]. 山东科学, 2008, 21(2):9-14.

[62] Arenillas A , Rubiera F , Pis J J . Simultaneous thermogravimetric–mass spectrometric study on the pyrolysis behaviour of different rank coals[J]. Journal of Analytical & Applied Pyrolysis, 1999, 50(1):31-46.

[63] 宋绍勇. 煤热解动学及其机理的实验研究[D]. 太原理工大学, 2002.

[64] 孙庆雷, 李文, 陈皓侃,等. 神木煤显微组分加氢热解的TG/MS研究[J]. 燃料化学学报, 2004, 32(6):647-651.

[65] 降文萍. 煤热解动力学及其挥发分析出规律的研究[D]. 太原理工大学, 2004.

[66] 王传格, 曾凡桂, 彭志龙, et al. 应用分布活化能模型分析伊敏褐煤丝炭腐植酸热解及氢气生成动力学[J]. 物理化学学报, 2012(1):25-36.

[67] 白宗庆, 陈皓侃, 李文, et al. 热重-质谱联用研究焦炭在甲烷气氛下的热行为[J]. 燃料化学学报, 2005, 33(4):426-430.

[68] 曾凡桂, 贾建波. 霍林河褐煤热解甲烷生成反应类型及动力学的热重-质谱试验与量子化学计算[J]. 物理化学学报, 2009, 25(6):1117-1124.

[69] 王传格. 煤显微组分热解甲烷、氢气生成动力学及机理[D]. 太原理工大学, 2006.

[70] 王传格, 曾凡桂. 神东煤镜质组和惰质组热解甲烷生成反应类型分析[J]. 太原理工大学学报, 2011, 42(3):241-247.

[71] 李美芬, 曾凡桂, 孙蓓蕾,等. 低煤级煤热解H\_2生成动力学及其与第一次煤化作用跃变的关系[J]. 物理化学学报, 2009, 25(12):2597-2603.

[72] 王民, 董奇, 卢双舫, et al. 松辽盆地沙河子组煤岩TG-MS实验产物特征及动力学分析[J]. 煤炭学报, 2012, 37(7):1150-1155.

[73] 范冬梅, 朱治平, 吕清刚. 热质联用研究烟煤热解气体释放特性[J]. 煤炭转化, 2014, 37(1).

[74] Han F, Meng A, Li Q, et al. Thermal decomposition and evolved gas analysis (TG-MS) of lignite coals from Southwest China[J]. Journal of the Energy Institute, 2016, 89(1):94-100.

[75] Duin A C T V , Dasgupta S , François Lorant, et al. ReaxFF: A Reactive Force Field for Hydrocarbons[J]. The Journal of Physical Chemistry A, 2001, 105(41):9396-9409.

[76] 刘连池. ReaxFF反应力场的开发及其在材料科学中的若干应用[D]. 上海交通大学, 2012.

[77]Zheng M, Wang Z, Li X, et al. Initial reaction mechanisms of cellulose pyrolysis revealed by ReaxFF molecular dynamics[J]. Fuel, 2016, 177(AUG):130-141.

[78] 刘健, 李晓霞, 郭力, et al. 反应分子动力学(ReaxFF MD)模拟结果分析工具VARxMD[J]. 计算机与应用化学, 2014, 31(6).

[79] Castro-Marcano F , Kamat A M , Russo M F , et al. Combustion of an Illinois No. 6 coal char simulated using an atomistic char representation and the ReaxFF reactive force field[J]. Combustion and Flame, 2012, 159(3):1272-1285.

[80] Salmon E , Duin A C T V , François Lorant, et al. Early maturation processes in coal. Part 2: Reactive dynamics simulations using the ReaxFF reactive force field on Morwell Brown coal structures[J]. Organic Geochemistry, 2009, 40(12):1195-1209.

[81] Mingjie Gao, Xiaoxia Li, Li Guo. Pyrolysis simulations of Fugu coal by large-scale ReaxFF molecular dynamics [J]. Fuel Processing Technology, 2018, 178:197-205.

[82] Dikun H , Liang L , Shu Z , et al. Effect of cooling rate on the reaction of volatiles from low-rank coal pyrolysis: Molecular dynamics simulations using ReaxFF[J]. Fuel Processing Technology, 2018, 178:133-138.

[83] HONG Dikun, GUO Xin. Molecular dynamics simulations of Zhundong coal pyrolysis using reactive force field[J],Fuel, 2017, 210:58-66.

[84] Bhoi S , Banerjee T , Mohanty K . Molecular dynamic simulation of spontaneous combustion and pyrolysis of brown coal using ReaxFF[J]. Fuel, 2014, 136:326-333.

[85] Chen B , Diao Z J , Zhao Y L , et al. A ReaxFF molecular dynamics (MD) simulation for the hydrogenation reaction with coal related model compounds[J]. Fuel, 2015, 154(5):114-122.

[86] Zheng M , Li X , Guo L . Algorithms of GPU-enabled reactive force field (ReaxFF) molecular dynamics[J]. Journal of Molecular Graphics & Modelling, 2013, 41(2):1-11.

[87] Mo Z , Xiaoxia L , Li G . Investigation of N behavior during coal pyrolysis and oxidation using ReaxFF molecular dynamics[J]. Fuel, 2018, 233:867-876.

[88] Castro-Marcano F, Russo M F , Van Duin A C T , et al. Pyrolysis of a large-scale molecular model for Illinois no. 6 coal using the ReaxFF reactive force field[J]. Journal of Analytical and Applied Pyrolysis, 2014, 109:79-89.

[89] Hanhui Jin, Bonan Xu, Hanqing Li, Xiaoke Ku, Jianren Fan. Numerical investigation of coal gasification in supercritical water with the ReaxFF molecular dynamics method[J],International Journal of Hydrogen Energy, 2018, 205:13-24

[90] Wang H , Feng Y , Zhang X , et al. Study of coal hydropyrolysis and desulfurization by ReaxFF molecular dynamics simulation[J]. Fuel, 2015, 145:241-248.

[91] Guang-Yue Li , Jun-Xia Ding , Hang Zhang , Cai-Xia Hou , et al. ReaxFF simulations of hydrothermal treatment of lignite and its impact on chemical structures[J]. Fuel, 2015, 154:243-251.

[92] Liu J , Li X , Guo L , et al. Reaction analysis and visualization of ReaxFF molecular dynamics simulations[J]. Journal of Molecular Graphics and Modelling, 2014, 53:13-22.

[93] Ying-Ying Li , Guang-Yue Li , Hang Zhang , et al. ReaxFF study on nitrogen-transfer mechanism in the oxidation process of lignite[J]. Fuel, 2017, 193:331-342

[94] 韩峰, 张衍国, 蒙爱红, et al. 云南褐煤结构的FTIR分析[J]. 煤炭学报, 2014, 39(11).

[95] 冯杰, 李文英, 谢克昌. 傅立叶红外光谱法对煤结构的研究[J]. 中国矿业大学学报, 2002, 31(5).

[96] 张科, 姚素平, 胡文瑄, et al. 煤红外光谱的精细解析及其煤化作用机制[J]. 煤田地质与勘探, 2009, 37(6):8-13.

[97] 郑庆荣, 曾凡桂, 张世同. 中变质煤结构演化的FT-IR分析[J]. 煤炭学报, 2011, 36(3):481-486.

[98] 贾建波, 王颖, 李风海, et al. 神东煤镜质组结构模型红外光谱的量子化学计算[J]. 光谱学与光谱分析, 2014, 34(1).

[99] 梁虎珍, 王传格, 曾凡桂, et al. 应用红外光谱研究脱灰对伊敏褐煤结构的影响[J]. 燃料化学学报, 2014, 42(2).

[100] 秦育红, 赵清艳, 赵永姣. 不同煤阶煤的吡啶抽提FTIR谱研究[J]. 煤化工, 2005, 33(1).

[101] 黄红英, 尹齐和. 傅里叶变换衰减全反射红外光谱法(ATR-FTIR)的原理与应用进展[J]. 中山大学研究生学刊(自然科学.医学版), 2011(1):20-31.

[102] 朱学栋, 朱子彬, 韩崇家, et al. 煤中含氧官能团的红外光谱定量分析[J]. 燃料化学学报, 1999(4):335-339.

[103] 宋昱, 朱炎铭, 李伍. 东胜长焰煤热解含氧官能团结构演化的13 C-NMR和FT-IR分析[J]. 燃料化学学报, 2015, 43(5):519-529.

[104] 秦志宏, 袁新华, 宗志敏,等. 用XRD,TEM和FTIR研究镜煤在CS2—N—甲基—2—吡咯烷酮混合溶剂中的溶解行为[J]. 燃料化学学报, 1998(3):275-279.

[105] JoséV. Ibarra, Mu?Oz E , Moliner R . FTIR study of the evolution of coal structure during the coalification process[J]. Organic Geochemistry, 1996, 24(6-7):0-735.

[106] 张卫, 曾凡桂. 中等变质程度煤中羟基的红外光谱分析[J]. 太原理工大学学报, 2005, 36(5):545-548

[107]

[108] 徐秀峰, 张蓬洲. 用XPS表征氧、氮、硫元素的存在形态[J]. 煤炭转化, 1996(1):72-77.

[109] Frost D C, Wallbank B, Leeder W R. Chapter 11 – X-Ray Photoelectron Spectroscopy of Coal and Coal Related Problems[J]. Analytical Methods for Coal & Coal Products, 1978, 36(1):349-376.

[110] Bo W U, Hao-Quan H U, Zhao Y P, et al. XPS analysis and combustibility of residues from two coals extraction with sub-and supercritical water[J]. 燃料化学学报, 2009, 37(4):385-392.

[111] 常海洲, 王传格, 曾凡桂, et al. 不同还原程度煤显微组分组表面结构XPS对比分析[J]. 燃料化学学报, 2006, 34(4):389-394.

[112] 段旭琴, 王祖讷. 煤显微组分表面含氧官能团的XPS分析[J]. 辽宁工程技术大学学报(自然科学版), 2010, 29(3).

[113] Gorbaty M L, George G N, Kelemen S R. Direct determination and quantification of sulphur forms in heavy petroleum and coals : 2. The sulphur K edge X-ray absorption spectroscopy approach[J]. Fuel, 1990, 69(8):945-949.

[114]杨卉艳. 微生物法脱除煤中有机氮研究[D]. 太原理工大学, 2005.

[115] Pietrzak R , Grzybek T , Wachowska H . XPS study of pyrite-free coals subjected to different oxidizing agents[J]. Fuel, 2007, 86(16):2616-2624.

[116] Grzybek T , Pietrzak R , Wachowska H . X-ray photoelectron spectroscopy study of oxidized coals with different sulphur content[J][J]. Fuel Processing Technology, 2002, 77(1):1-7.

[117] Gardner S D, Singamsetty C S K, Booth G L, et al. Surface characterization of carbon fibers using angle-resolved XPS and ISS[J]. Carbon, 1995, 33(5):587-595.

[118] 姚明宇, 刘艳华, 车得福. 宜宾煤中氮的形态及其变迁规律研究[J]. 西安交通大学学报, 2003, 37(7):759-763.

[119] 陈保国. X射线衍射(XRD)在研究煤结构中的应用[J]. 现代商贸工业, 2014(3):195-196.

[120] 张代钧, 鲜学福. 煤结构的X射线分析[J]. 西安科技大学学报, 1990(3):42-49.

[121] 煤及半焦的XRD结构分析[J]. 河南城建学院学报, 2014, 23(1):32-37.

[122] 张小东, 孔令菲, 秦勇, et al. 龙口褐煤萃取后微晶结构的XRD与HRTEM研究[J]. 煤炭学报, 2013, 38(06):1025-1030.

[123] 李美芬, 曾凡桂, 齐福辉,等. 不同煤级煤的Raman谱特征及与XRD结构参数的关系[J]. 光谱学与光谱分析, 2009, 29(9):2446-2449.

[124] 李霞, 曾凡桂, 王威, et al. 低中煤级煤结构演化的XRD表征[J]. 燃料化学学报, 2016, 44(7).

[125] Yoshida T , Maekawa Y . Characterization of coal structure by CP/MAS carbon-13 NMR spectrometry[J]. Fuel Processing Technology, 1987, 15(none):385-395.

[126] 叶朝辉, 李新安. 煤的固体高分辨~(13)C-NMR谱[J]. 科学通报, 1985, 30(20):1545-1545.

[127] Ü Lille, Heinmaa I , Pehk T . Molecular model of Estonian kukersite kerogen evaluated by 13C MAS NMR spectra☆[J]. Fuel, 2003, 82(7):799-804.

[128] Okolo G N , Neomagus H W J P , Everson R C , et al. Chemical–structural properties of South African bituminous coals: insights from wide angle XRD–carbon fraction analysis, ATR–FTIR, solid state 13C NMR, and HRTEM techniques[J]. Fuel, 2015, 158:779-792.

[129] Solum M S, Pugmire R J, Grant D M. Carbon-13 solid-state NMR of Argonne-premium coals[J]. Energy & Fuels, 1989, 3(2):187-193.

[130] Suggate R P , Dickinson W W . Carbon NMR of Coals: The Effects of Coal Type and Rank[J]. International Journal of Coal Geology, 2004, 57(1):1-22.

[131] Kalaitzidis S , Georgakopoulos A , Christanis K , et al. Early coalification features as approached by solid state 13C CP/MAS NMR spectroscopy[J]. Geochimica Et Cosmochimica Acta, 2006, 70(4):0-959.

[132] Mathews J P , Duin A C T V , Chaffee A L . The utility of coal molecular models[J]. Fuel Processing Technology, 2011, 92(4):718-728.

[133] Kalaitzidis S , Georgakopoulos A , Christanis K , et al. Early coalification features as approached by solid state 13C CP/MAS NMR spectroscopy[J]. Geochimica Et Cosmochimica Acta, 2006, 70(4):0-959.

[134] 葛涛, 蔡川川. 不同密度炼焦煤中有机硫的 XPS 研究[J]. 安徽理工大学学报（自然科学版）, 2015(3).

[135] 代世峰, 任德贻, 宋建芳,等. 应用XPS研究镜煤中有机硫的存在形态[J]. 中国矿业大学学报, 2002, 31(3):225-228.

[136] 陈鹏. 用XPS研究兖州煤各显微组分中有机硫存在形态[J]. 燃料化学学报, 1997(3):238-241.

[137] 董夔. 太原西山西铭8号煤大分子结构构建及甲烷吸附机理研究[D]. 2015.

[138] 程丽媛. 屯兰8号煤大分子结构模型及其热解过程中氢气与甲烷生成动力学[D]. 太原理工大学, 2015.

[139] 马延平. 柳林3#煤的超分子构建及分子模拟[D]. 太原理工大学, 2012.

[140] 李鹏鹏. 杜儿坪2号煤结构模型构建及其分子模拟[D]. 太原理工大学, 2014.

[141] Mathews J P , Duin A C T V , Chaffee A L . The utility of coal molecular models[J]. Fuel Processing Technology, 2011, 92(4):718-728.

[142]王莹. 计算机分子模拟中并行计算的研究[D]. 北京化工大学, 2001.

[143] 基于量子化学方法的煤氧吸附特性模拟实验研究[D]. 西安科技大学, 2011.

[144] 文玉华, 文玉华, 朱如曾, et al. 分子动力学模拟的主要技术[J]. 力学进展, 1900, 33(1).

[145] 唐赟, 李卫华, 盛亚运. 计算机分子模拟——2013年诺贝尔化学奖简介[J]. 自然杂志, 2013, 35(6):408-415.

[146]李卓谡, 赵玉洁, 贾晓娜, et al. 分子动力学计算机模拟技术进展[J]. 机械管理开发, 2008, 23(2):174-176.

[147] 王长安, 辛海会, Watson J K , et al. 煤焦O2/CO2燃烧反应性及结构演化的分子\\模拟研究[J]. 工程热物理学报, 2016.

[148] 王艺峰, 程时远, 王世敏, et al. 高分子材料模拟中的分子力学法和力场[J]. 高分子材料科学与工程, 2003, 19(1):10-14.

[149] 黄世强, 朱申敏, 程时远. 聚合物分子模拟中的力场[J]. 高分子材料科学与工程, 1999, 15(4).

[150] 王长安, 车得福. 耦合堆垛与孔径分布的高碱金属煤焦分子建模方法[J]. 西安交通大学学报, 2017(9).

[151] 煤中有机硫微波脱除的量子化学模拟与实验研究[D]. 中国矿业大学, 2016.

[152] 褐煤结构的分子动力学模拟及量子化学研究[D]. 太原理工大学, 2004.

[153] 冯晓琴, 任福德, 曹端林. Gaussian量子化学模拟对芳烃硝化机理的探索[J]. 大学化学, 2008, 23(1):37-39.

[154] 陶旭梅, 孙晋良, 柳文杰, et al. CO2和H2合成甲醇的量子化学模拟[J]. 天然气化工(C1化学与化工）, 2013(3):57-61.

[155] 黎乐民, 刘俊婉, 金碧辉. 密度泛函理论[J]. 中国基础科学, 2007, 7(3):27-28.

[156] 沈尔忠, 杨忠志. 密度泛函理论下的分子电负性：Ⅲ.分子总能量的直接计算[J]. 化学学报, 1996(2):152-159.

[157] Niekerk D V , Mathews J P . Molecular dynamic simulation of coal–solvent interactions in Permian-aged South African coals[J]. Fuel Processing Technology, 2011, 92(4):729-734.

[158] 胡宗球. 键能的分子轨道理论研究 Ⅰ.理论公式[J]. 化学学报, 1998, 56(4):353-358.

[159] 唐诗雅, 傅尧, 郭庆祥. 铬族金属氢化物中M-H 键键能的从头计算[J]. 化学学报, 2012, 70(18):1923-1929.

[160] 陈阳亨, 冉鸣. 关于键解离能、键能、反应焓变的探讨[J]. 化学教育, 2017(17).

[161] Russo M F , Duin A C T V . Atomistic-scale simulations of chemical reactions: Bridging from quantum chemistry to engineering[J]. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2011, 269(14):1549-1554.

[162] CASTROMARCANO, Fidel, LOBODIN, et al. A molecular model for Illinois No. 6 Argonne Premium coal: Moving toward capturing the continuum structure[J]. Fuel, 2012, 95(1):35-49.

[163] 郑默. 基于GPU的煤热解化学反应分子动力学（ReaxFF MD）模拟[D]. 2015.

[164] 林蔚. 煤热解焦化和加氢脱硫的ReaxFF反应分子动力学分析[D]. 2016.

[165] 刘连池. ReaxFF反应力场的开发及其在材料科学中的若干应用[D]. 上海交通大学,2012.

[166] Zhong Q , Mao Q , Xiao J , et al. Sulfur removal from petroleum coke during high-temperature pyrolysis. Analysis from TG-MS data and ReaxFF simulations[J]. Journal of Analytical and Applied Pyrolysis, 2018:S0165237017311166.

[167] Li G Y , Wang F , Wang J P , et al. ReaxFF and DFT study on the sulfur transformation mechanism during the oxidation process of lignite[J]. Fuel, 2016, 181:238-247.

[168] Zhang J , Weng X , Han Y , et al. The effect of supercritical water on coal pyrolysis and hydrogen production: A combined ReaxFF and DFT study[J]. Fuel, 2013, 108:682-690.

[169] Ohrbach K H, Klusmeier W, Kettrup A. TG-DTA-MS Investigations of coal, and characterization of the volatile products released as a function of temperature[J]. Journal of Thermal Analysis, 1984, 29(1):147-152.

[170] 孟丽莉, 付春慧, 王美君, et al. 碱金属碳酸盐对褐煤程序升温热解过程中H2S和NH3生成的影响[J]. 燃料化学学报, 2012, 40(2).

[171] Dong-ke, Zhang. 低阶煤程序升温热解过程中钠、硅和硫间的相互作用[J]. 燃料化学学报, 2005, 33(5).

[172] 王志青, 白宗庆, 李文, et al. 常压程序升温热解-质谱系统在煤脱羧过程中的应用[J]. 分析化学, 2010, 38(3):393-396.

[173] 蔡连国, 刘文钊, 余剑, et al. 煤程序升温与等温热解特性及动力学比较研究[J]. 煤炭转化, 2012, 35(3).

[174] OHTSUKA, ZHIHENG, FURIMSKY. Effect of alkali and alkaline earth metals on nitrogen release during temperature programmed pyrolysis of coal[J]. Fuel, 1997, 76(14):1361–1367.

[175] Luo G , Yao H , Xu M , et al. Identifying modes of occurrence of mercury in coal by temperature programmed pyrolysis[J]. Proceedings of the Combustion Institute, 2011, 33(2):2763-2769.

[176] Boudou J P . Coal Desulfurization by Programmed-Temperature Pyrolysis and Oxidation[M]. 1990.

[177] Liu F R, Wen L I, Bao-Qing L I, et al. Sulfur transformation during pyrolysis of Zunyi coal by atmosphere pressure-temperature programmed reduction-mass spectrum[J]. Journal of Fuel Chemistry & Technology, 2008, 36(1):6-9.

[178] LIPINGCHANG. Effect of Operating Parameters on HCN and NH3 Release from Australian and Chinese Coals During Temperature-Programmed Pyrolysis[J]. Energy Sources, 2003, 25(7):10.

[179] Zhang D K. Interactions between sodium, silica and sulphur in a low-rank coal during temperature-programmed pyrolysis[J]. Journal of Fuel Chemistry & Technology, 2005, 33(5):513-519.

[180] Otero M, Dı́Ez C, Calvo L F, et al. Analysis of the co-combustion of sewage sludge and coal by TG-MS[J]. Biomass & Bioenergy, 2002, 22(4):319-329.

[181] Arenillas A, Pevida C, Rubiera F, et al. Characterisation of model compounds and a synthetic coal by TG/MS/FTIR to represent the pyrolysis behaviour of coal[J]. Journal of Analytical & Applied Pyrolysis, 2004, 71(2):747-763.

[182] Zhao Y, Haoquan H U, Jin L, et al. Pyrolysis behavior of vitrinite and inertinite from Chinese Pingshuo coal by TG–MS and in a fixed bed reactor[J]. Fuel Processing Technology, 2011, 92(4):780-786.

[183] 张妮, 曾凡桂, 降文萍. 中国典型动力煤种热解动力学分析[J]. 太原理工大学学报, 2005, 36(5):549-552.

[184] 降文萍. 煤热解动力学及其挥发分析出规律的研究[D]. 太原理工大学, 2004.

[185] Li W , Zhu Y . Structural Characteristics of Coal Vitrinite during Pyrolysis[J]. Energy & Fuels, 2014, 28(6):3645-3654.

[186] Wiktorsson L P , Wanzl W . Kinetic parameters for coal pyrolysis at low and high heating rates—a comparison of data from different laboratory equipment[J]. Fuel, 2000, 79(6):701-716.

[187] SOLOMON P. R, SERIO M. A, CARANGELO R. M, et al. Very rapid coal pyrolysis[J]. Fuel, 1986, 65(2):182-194.

[188] Swope W C, Ferguson D M. Alternative expressions for energies and forces due to angle bending and torsional energy[J]. Journal of Computational Chemistry, 1991, 13(5):585-594.

[189] Johansson M P, Olsen J. Torsional Barriers and Equilibrium Angle of Biphenyl: Reconciling Theory with Experiment.[J]. Journal of Chemical Theory & Computation, 2008, 4(9):1460.

[190] Schaumann T, Braun W, Wüthrich K. The program FANTOM for energy refinement of polypeptides and proteins using a Newton – Raphson minimizer in torsion angle space[J]. Biopolymers, 2010, 29(4-5):679-694.

[191] Benniston A C, Harriman A, Li P, et al. The effect of torsion angle on the rate of intramolecular triplet energy transfer.[J]. Physical Chemistry Chemical Physics Pccp, 2005, 7(21):3677-3679.

[192] 冯锡璋. 范德华能与配位键能之间的平衡——钇络合物中配位键长的综合模型[J]. 北京师范大学学报:自然科学版, 1987(2):58-60.

[193] Buhmann S Y, Dung H T, Kampf T, et al. Atoms near magnetodielectric bodies: van der Waals energy and the Casimir-Polder force[J]. Optics & Spectroscopy, 2005, 99(3):466-474.

[194] Simpson W T, Peterson D L. Coupling Strength for Resonance Force Transfer of Electronic Energy in Van der Waals Solids[J]. Journal of Chemical Physics, 1957, 26(3):588-593.

[195] Sawada T. A proposal to observe a strong Van der Waals force in low energy proton‐proton scattering[C]// 2008.

[196] 朱遵略, 马恒, 孙金锋. BH分子势能函数研究[J]. 原子与分子物理学报, 2006, 23(6):1092-1096.

[197] 朱正和, 俞华根. 分子结构与分子势能函数[M]. 科学出版社, 1997.

[198] 伍冬兰, 涂娟, 万慧军, et al. 外电场下BH分子势能函数[J]. 计算物理, 2014, 31(1):115-120.

[199] 刘国跃. 双原子分子势能函数的研究进展[J]. 绵阳师范学院学报, 2005, 24(5):46-51.

[200] 代亚, 胡匡民. 能量最低原理与物质结构、性质之间的内在联系[J]. 化学教育, 1984, 5(2):51-53.

[201] 吴孙富, 张道林. CH4与NH3稳定性的比较[J]. 化学教育, 2008, 29(5):74-74.

[202] 赵洁雯, 黄晓明, 李晓东. 基于热重质谱联用的沥青质燃烧特性分析[J]. 东南大学学报(自然科学版), 2014, 44(1):178-182.

[203] Di Blasi C , Signorelli G , Di Russo C , et al. Product Distribution from Pyrolysis of Wood and Agricultural Residues[J]. Industrial & Engineering Chemistry Research, 1999, 38(6):2216-2224.

[204] Behar F , Hatcher P G . Artificial Coalification of a Fossil Wood from Brown Coal by Confined System Pyrolysis[J]. Energy & Fuels, 1995, 9(6):984-994.

[205] Wang S , Liao Y , Luo Z . Mechanism Study of Cellulose Rapid Pyrolysis[J]. Industrial & Engineering Chemistry Research, 2004, 43(18):5605-5610.

[206] 张辰宇. 基于常见农林废弃生物质原料的热解技术及机理研究[D]. 北京化工大学, 2013.

[207] 张强. 生活垃圾热解气化处理工艺开发与过程模拟分析[D]. 2014.

[208] 程占军. 呋喃及其衍生物的变压力热解实验与模型研究[D]. 中国科学技术大学, 2014.

[209] 王传格. 低煤级煤不同化学组分结构及其热解主要气态产物生成机制[D]. 2012.

[210] 李美芬. 低煤级煤热解模拟过程中主要气态产物的生成动力学及其机理的实验研究[D]. 太原理工大学, 2009.

[211] 刘生玉. 中国典型动力煤及含氧模型化合物热解过程的化学基础研究[D]. 太原理工大学, 2004.

[212] Li Z K , Wei X Y , Yan H L , et al. Insight into the structural features of Zhaotong lignite using multiple techniques[J]. Fuel, 2015, 153:176-182.

[213] 潘婵婵, 刘霞, 霍威, et al. 煤气化细灰及其原煤的热解特性与官能团特征[J]. 化工学报, 2015, 66(4):1449-1458.

[214] Peng Xia, Fangui Zeng\*, Xiaoxia Song, Kunjie Li, Jin Wang, Shaosheng Feng, Beilei Sun. Geologic structural controls on coalbed methane content of the No. 8 coal seam, Gujiao area, Shanxi, China. Applied Ecology and Environmental Research, 2017, 15(1): 51-68.

[215] Peng Xia, Fangui Zeng\*, Xiaoxia Song, Yanjun Meng, Kunjie Li, Jin Wang, Beilei Sun. Structural block division for further deep research in coalbed methane development in the Gujiao area, Xishan coalfield, North China. Arabian Journal of Geosciences, 2016, 9(18), 713.

[216] Peng Xia, Fangui Zeng\*, Xiaoxia Song. Parameters controlling high-yield coalbed methane vertical wells in the B3 area, Xishan coal field, Shanxi, China. Energy Exploration & Exploitation, 2016, 34(5): 711-734.

[217] 张义军. C4系列烷烃和烯烃的热解实验及动力学模型研究[D]. 中国科学技术大学, 2013.

[218] 范冬梅, 张海霞, 朱治平, et al. 一种褐煤热解煤焦的CO2气化反应特性[J]. 煤炭转化, 2012, 35(4):20-25.