

Research on Carbon Emission Reduction Performance of CCUS Projects in China Under the Background of Carbon Neutralization

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Abstract: This paper uses data envelopment (DEA) model to measure the carbon emission reduction performance of CCUS demonstration projects in China. The carbon reduction performance is analyzed from the aspects of technical efficiency and scale efficiency, and the carbon reduction performance level, low efficiency reasons and improvement focus of each demonstration project are evaluated and analyzed. It is found that the carbon reduction performance is affected by projects in China is relatively low at the present stage, and the emission reduction performance is affected by project size, financing level and industrial process. The scale of CCUS project does not match the input-output, so resource allocation should be adjusted under the support of technology. While vigorously promoting CCUS project construction under the guidance of carbon neutrality goal, attention should be paid to scale efficiency and operation and maintenance management of the project, so as to promote the smooth implementation of technological carbon emission reduction path.

Keywords Carbon neutrality; Carbon Capture, Utilization and Storage (CCUS); Carbon emission reduction efficiency; DEA

INTRODUCTION

The carbon neutral target points out the direction for China to respond to climate change in the medium and long term, and is a specific time target proposed since China is committed to developing a low-carbon economy. China's energy structure is still dominated by fossil fuels and cannot be changed in the short term. This reality highlights the importance of process emission reduction, that is, the choice of emission reduction path. Technological innovation and progress has always been an inexhaustible driving force to promote the development of low-carbon economy in China. According to the 5th Assessment report of the Intergovernmental Panel on Climate Change (IPCC) and the International Energy Agency (IEA), to achieve the goal of controlling the global temperature rise within 2° C by the end of this century. In the best case, up to 14% of CO₂ reduction needs to be achieved by CCUS technology. According to the ENERGY Technology Outlook 2020 report released by the IEA, OVER the next 50 years, CCUS can afford to reduce emissions in the power and industrial sectors by nearly 600 gigatons, equivalent to 17 years of human CO₂ emissions. As a new development trend of carbon capture and storage (CCS) technology, CCUS has once become a hot research topic in the academic circles at home and abroad in the era of climate economy.

Fan Ying et al. [Fan Ying et al., 2017] evaluated the application status of carbon capture and storage technology, discussed the carbon reduction potential

technical suggestions for future development and promotion. Li Xiaochun and Zhang Jiutian[Li Xiaochun et al., 2018] evaluated the implementation of CCUS based on the 2011 Version of China's carbon capture, Utilization and storage technology roadmap, analyzed the problems existing in the current development of CCUS in China and put forward relevant suggestions. DEA was first proposed by Charnes and Cooper [Charnes and Cooper, 1978] as a non-parametric analysis method, and was applied to measure the efficiency of carbon emission reduction. Later, some scholars used DEA to evaluate the economic benefits of energy utilization and the efficiency of carbon emission reduction. Taking GDP growth as expected output and CO2 emission and energy consumption as unexpected output, DEA model was used to explore the input-output relationship among the three. The study of Lozano et al. [Lozano et al., 2008] proved that carbon emission reduction and GDP growth could be realized simultaneously. Wang Yan and Su Yiji [Wang Yan and Su Yiji, 2020] explored the influencing factors of China's regional energy saving and emission reduction efficiency from the green perspective with DEA model, and conducted Tobit regression analysis on the impact of industrial structure on emission reduction efficiency. Hang Qingyu et al. [Zhang Qingyu et al., 2016] applied the improved DEA model to evaluate the carbon emission reduction efficiency of 42 departments in Beijing, analyzed the causes of invalid DEA units, and finally put forward targeted

of the technology project, and put forward policy and

suggestions for the optimization and upgrading of industrial structure. China's National Development and Reform Commission has explicitly mentioned that the industries carrying out CCUS pilot projects involve thermal power, coal chemical industry, cement and steel industry, which will be the key fields of CCUS application in the future for a long time. Therefore, this paper explores the carbon reduction performance of China's current CCUS technology against the background of carbon neutrality, which is conducive to the improvement and promotion of the technology. In order to give full play to the contribution of carbon neutral emission reduction targets.

CARBON NEUTRALITY AND EMISSION REDUCTION PERFORMANCE

Carbon neutrality refers to the use of afforestation, technological innovation, energy conversion and other forms of energy saving and emission reduction to offset the carbon dioxide generated in a certain period of time, so as to achieve relative "zero emissions". which is another extension of low-carbon economy. China's carbon dioxide emissions account for about 30% of the world's total, more than the combined emissions of the United States, the European Union and Japan. It only takes 30 years from "carbon peak" to "carbon neutral", so the time is tight and the task is heavy. Published in our country, the carbon dioxide capture, utilization and storage (CCUS) report (2019) clearly pointed out that in carbon dioxide capture, utilization and storage (CCUS) technique is currently the only one to realize near-zero emissions of fossil energy use technology, not an overnight clean energy transformation, must clean energy and the coordinated development of low-carbon technologies, To achieve low-carbon sustainable development.

As a key area of carbon emission reduction, enterprises should take into account profits and benefits while performing carbon reduction responsibilities. The investment in CCUS technology is bound to increase costs, and CCUS technology itself is a process of multi-input and multi-output. Compared with CCS technology, CCUS adds "Utilization". The captured CO₂ can be used in geology, chemical industry, biology and other fields, such as CO2 flooding, production of fertilizer, improve salt and alkali water quality and other industrial benefits. Through the continuous improvement of technology to improve the efficiency of carbon dioxide emission reduction, while reducing the cost of technology operation. Through exploring the carbon reduction performance of China's currently mature CCUS demonstration projects, the ways to improve CCUS performance are explored. Performance, that is, the combination of performance and efficiency,

performance is performance, reflects the profit target: Efficiency is efficiency. Carbon reduction performance is a concept with multiple objectives, which not only covers the carbon emission efficiency studied by most scholars, but also includes the consideration of project economic benefits. Based on the background of low-carbon economy, under the goal of carbon neutrality, we should pay attention to the performance of carbon emission reduction, explore energy-saving and emission reduction paths that are more in line with the current energy situation of China, and promote the deployment of CCUS in the national high energy consumption industries, so as to achieve the goal of carbon neutrality in a better and faster way.

STUDY DESIGN

DEA performance measurement model

Data Envelopment analysis (EDA). It is a nonparametric efficiency evaluation method based on relative efficiency. Using DEA method to evaluate the efficiency has a great advantage, don't need to know the particular form of production function, also do not need a unified unit of each input and output indicators of index number has no specific restrictions, at the same time this method is not affected by a variety of subjective factors, also do not have to give every index weight, relying only on the relative effectiveness of input and output indicators of decision making units to assess, Then the improvement direction of DMU which is not effective is proposed. CCUS is a multiple input multiple output low carbon technology projects, and the function relationship between the input and output is difficult to determine, so this article use the DEA method, according to the construction of the demonstration project funding, carbon reduction performance on the basis of the distance between the output and the production frontier, the current domestic CCUS demonstration project of CO₂ emission reduction performance measure.

Based on different production possibility sets, DEA can be divided into C^2R model with constant returns to scale and BC^2 model with variable returns to scale, with different assumptions. This paper intends to analyze CCUS projects in the process of carbon reduction the shortage of input and output efficiency and therefore the BC^2 model of DEA method, it is concluded that the comprehensive efficiency of the C^2R model on further decomposition, in-depth analysis of its pure technical efficiency and scale efficiency, and through the analysis with the distance of the production frontier DEA invalid input redundancy and output deficiency of project status, In order to provide reference suggestions for CCUS projects with low carbon reduction performance.

The specific DEA model is as follows: $\min: \theta$

indicators

$$\begin{bmatrix} \sum_{j=1}^{n} \lambda_{j} \chi_{j} + s^{T} = \theta \chi_{0} \\ \sum_{j=1}^{n} \lambda_{j} \gamma_{j} - s^{T} = \gamma_{0} \\ \text{st.} \quad \sum_{j=1}^{n} \lambda_{j} = 1 \qquad (1) \\ \lambda \ge 0, \ j = 1, 2., ..., n \\ s^{T} \ge 0, \ s^{T} \ge 0 \end{bmatrix}$$

In formula (1), Θ indicates the planned target value, λ_j is the planning decision variable, χ_j is the factor input of DMU_j , y_j is the factor output of DMU_j , $s^- \ s^+$ is the vector of relaxation variables.

This paper uses DEA method,
$$\sum_{j=1}^{n} \lambda_j = 1 (\lambda > 0)$$

Build the BC² model, when $\theta = 1$, and $s^{\dagger} = 0$, $s^{\dagger} = 0$, It indicates that the decision making unit is effective with strong DEA; when $\theta = 1$, $s^{+} \neq 0$ or $s^{-} \neq 0$, The decision unit is DEA weakly effective; when $\theta < 1$. The decision unit DEA is invalid.

Data source and Index selection

At present, there are 21 CCUS projects in operation in China, and the remaining 17 CCUS investment construction projects bring benefits through CO₂-EOR (enhanced gas recovery), marketing and chemical production, except the 4 demonstration projects of CO₂ salt water sealing layer that do not generate profits. Considering the purpose of combining the analysis of emission reduction efficiency and economic benefit of CCUS project in this paper, four CO₂ salt water sealing projects that do not generate income are removed.

In the selection of input and output index, combined with the purpose of this article explores, on CCUS emissions performance measure of the project, at the same time be able to more fully reflect the input and output of each reduction projects to serve the economic benefit evaluation for capacity and efficiency of carbon dioxide emission reduction, and in ensuring that index data can be obtained on the basis of selecting an economic indicators - carbon capture cost, A scale index -- project capital input; In previous studies, CO_2 reduction was mostly regarded as undesired output, that is, the larger the value, the better.

However, this paper believes that CO_2 reduction can be converted into CO_2 capture, which can be regarded as expected output. The utilization of CO_2 can obtain benefits through oil displacement recovery, chemical production and biological utilization, so CO_2 capture and utilization are selected as two output indicators. The specific input-output indicators are as follows: Table 1 Carbon emission reduction performance

evaluation index system of CCUS projects			
Туре	The index	Variable symbol	
Input indicators	CO ₂ Capture Costs	<i>X</i> ₁	
	Capital Input	<i>X</i> ₂	
	CO ₂ Utilization	Y_1	
Output	CO ₂ Containme	V	

 $\frac{\text{CO}_2\text{Capture}}{\text{In the application of DEA analysis, the number of decision making units and input-output indicators should meet the conditions in Formula (2) :$

 Y_2

 Y_3

 $n \ge max \{ m \times s, 3 (m + s) \}$ (2)

nt

Where, n is the number of decision making units, m is the number of input indicators, and s is the number of output indicators. In this paper, 2 input indicators, 2 output indicators and 17 decision units are selected, which meet the quantity requirements of the above indicators.

The sequestered carbon dioxide returned to the surface with oil extraction and the CO₂ released during the operation of the project exist in all projects, so the impact of these two aspects is not considered. Under the assumption that the capture cost is fixed, oil price and carbon price have a greater impact on the profit of CO₂ utilization. In order to be consistent, this paper does not distinguish oil displacement, sale and other industrial profit methods, and selects CARBON dioxide utilization as Y₁, which represents the output index to measure the economic benefits of CCUS. The data in this paper are derived from China CCUS Development Roadmap (2019), China CARBON Dioxide Capture, Utilization and Storage (CCUS) Report (2019), and public data collection of CCUS demonstration projects.

MEASUREMENT AND ANALYSIS OF EMISSION REDUCTION PERFORMANCE OF CCUS PROJECTS

The names of CCUS demonstration projects are listed in abbreviation, and the specific names and order are shown in Table 2:

Table 2Name and sec	uence of CCUS projects
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Table 21 value and sequence of CC	ies projects
The project	Concise
Gaobeidian Power Plant	
Project	HNGBD
Huaneng Shidongkou	
Project	HNSDK
Chongqing Shuanghuai	
Power Plant Project	ZDTCQSH
Shengli Oilfield Project	SLYT
Tianjin Beitang Power Plant	
Project	TJBT
Beijing Gaojing Thermal	
Power Plant Project of	
Datang Group	DTGJ
Yanchang Petroleum Coal	
chemical engineering	
Project in northern Shaanxi	YCSYSB
	HK35
•	
5	XJDHKLMY
5	ZSHZY
	DQXSJ
1 ~	
	ZSHQLHG
5	ZSYJLCL
0	TWSN
	HLBMS
	HRHF
Huadong Ulffield - Jiangsu	
	UDICUN
Project	HDJSHY
	The projectHuaneng BeijingGaobeidian Power PlantProjectHuaneng ShidongkouProjectChongqing ShuanghuaiPower Plant ProjectShengli Oilfield ProjectTianjin Beitang Power PlantProjectBeijing Gaojing ThermalPower Plant Project ofDatang GroupYanchang Petroleum Coalchemical engineeringProject in northern Shaanxi35 MW oxygen-richCombustion Project ofHuazhong University ofScience and TechnologyXinjiang Dunhuang Petro-Karamay Methanol PlantProjectSinopec Zhongyuan OilfieldProjectDaqing Oilfield-XushenjiuNatural Gas Plant ProjectSinopec Qilu ChemicalProjectCNPC Jilin OilfieldChangling Natural Gas PlantProjectCanch Group-BaimashanCement Plant ProjectChina Resources HaifengCarbon capture Test ProjectHuadong Oilfield - JiangsuHuayang Liquid carbonProject

In this paper, Deap2.1 software is used to evaluate the carbon reduction performance of 17 decision units, and the DEA value of carbon reduction performance of each CCUS demonstration project in China is obtained, as shown in Table 3.

Table 3 DEA value of CO ₂ emission reduction					
efi	efficiency of CCUS projects				
	Comp	Pure		Scale	
Project	rehen	technic	Scale	reward	
	sive	al		lewalu	
HNGBD	0.075	1	0.075	↑	
HNSDK	1	1	1		
ZDTCQSH	0.125	0.196	0.638	↑	
SLYT	0.825	0.878	0.939	\downarrow	
TJBT	0.786	0.802	0.979	↑	
DTGJ	0.067	1	0.067	↑	

YCSYSB	1	1	1	
HK35	0.465	0.696	0.668	\downarrow
XJDHKLMY	0.87	1	0.87	↑
ZSHZY	1	1	1	
DQXSJ	1	1	1	
ZSHQLHG	0.769	0.817	0.941	\downarrow
ZSYJLCL	1	1	1	
TWSN	0.078	0.37	0.211	↑
HLBMS	0.404	0.423	0.956	↑
HRHF	0.147	0.16	0.919	\downarrow
HDJSHY	0.687	1	0.687	↑

The carbon dioxide reduction performance of domestic CCUS demonstration projects is analyzed from the changes of comprehensive efficiency, pure technical efficiency, scale efficiency and scale return.

Comprehensive efficiency analysis

Comprehensive efficiency, also known as technical efficiency, refers to the technical efficiency without considering the return on scale. If the comprehensive efficiency value is 1, it means that the effective frontier formed by the decision making unit is unchanged and the technology is effective. According to Table 2, only 5 of the 17 CCUS demonstration projects have achieved DEA effectiveness, including Huaneng Shidongkou Project, Yanchang Petroleum Shanbei Coal chemical Project, Sinopec Zhongyuan Oilfield project, Daqing Oilfield-Xushenjiu Natural Gas Plant project, and CNPC Jilin Oilfield-Changling Natural Gas Plant project. Among the above 5 projects with comprehensive efficiency of 1, except Huaneng Shidongkou Project, which is a capture project relying on power plant construction, the rest are all carbon capture projects operated on the basis of oil field. The effective carbon emission reduction of Shidongkou Power Plant project can provide reference for the construction of other similar projects. Among the other 12 carbon capture projects that fail to reach DEA effectiveness, the comprehensive efficiency DEA values of each demonstration project vary greatly, and the lowest value is 0.067 of Beijing Gaojing Thermal Power Plant project of Datang Group. In addition, the comprehensive efficiency of Huaneng Beijing Gaobeidian Power Plant project is 0.075, Taiwan Cement project is 0.078, CHONGQING Shuanghuai Power Plant project of China Power Investment Corporation is 0.125, and Carbon capture test platform of China Resources Haifeng is 0.147, all of which are at a low level.

On the whole, the carbon emission reduction performance of China's carbon capture, utilization and storage projects is generally low. Under the current capital investment level, only a few 5 projects have achieved DEA effective carbon emission reduction, indicating that there is still a large space for improvement in resource allocation and utilization of CCUS demonstration projects in China.

Analysis of pure technical efficiency and scale efficiency

Pure technical efficiency and scale efficiency are further split of comprehensive efficiency, Pure technical efficiency \times Scale efficiency = Comprehensive efficiency. Pure technical efficiency can represent the optimal level of project resource allocation, while scale efficiency represents the economic output level of resource input scale. As can be seen from the two efficiency values in Table 2, the resource allocation level and economic output level of carbon capture utilization and storage technology in China differ greatly in terms of carbon emission reduction.

First of all, pure technical efficiency is an efficiency assessment without considering the loss of factor utilization. It can reflect the efficiency generated by the operation management and technology application of carbon capture projects. According to the pure technical efficiency value in Table 2, at the current carbon capture utilization and storage technology level, 9 of the 17 demonstration projects have achieved DEA effectiveness. Huaneng Beijing gaobeidian power plant project, huaneng Shi Dongkou takai has retired, datang group, Beijing thermal power plant projects, prolong oil coal chemical projects of shaanxi, xinjiang oil - dunhuang karamay methanol plant projects, sinopec zhongyuan oilfield, daqing oilfield - xu deep nine - changling gas plant project, petrochina jilin oilfield gas plant project, east China oilfield in jiangsu Yang hua liquid carbon items This shows that the resource allocation structure of these 9 projects is good. the resource input is effective, and CCUS technology itself is not a problem in China. At the same time, there are four projects with low pure technical efficiency due to unreasonable resource allocation, among which the lowest 0.160 is the Carbon capture test project of China Resources Haifeng.

Secondly, scale efficiency is the production efficiency affected by the scale of resource input and output, which can reflect the efficiency difference between the existing scale and the optimal scale. In 17 projects with five CCUS projects reached the scale of DEA effective, huaneng Shi Dongkou project, prolong oil shanbei coal chemical projects, sinopec zhongyuan oilfield, daqing oilfield - xu deep nine - changling gas plant project and petrochina jilin oilfield gas plant project, the five project in technology and management level under the premise of a certain, The scale of its resource input is effective. Obviously, it is the effective scale of these five projects that determines the effective comprehensive efficiency. The scale efficiency value of the remaining 12 projects is less than 1, and the production scale and financial constraints may lead to the failure of the project to operate at the optimal scale.

Input-output analysis

According to Table 3, the overall CO_2 emission reduction performance of CCUS demonstration

projects in China is not effective, and the comprehensive efficiency is only 0.606. The two values of pure technical efficiency and scale efficiency are similar, and the lower value is scale efficiency value 0.762, indicating that the lower carbon emission performance of projects is mainly due to scale factor. Under the current low-carbon technology and management system, China's carbon capture projects are mostly inefficient in emission reduction due to the unreasonable scale of projects. Therefore, the reform should focus on improving the economies of scale of projects.

Table 4 DEA mean value of CO₂ emission reduction efficiency of CCUS projects

efficiency of CCOS projects			
	The	Pure	The scale
	comprehensiv e efficiency	technical efficiency	efficiency
The average	0.606	0.785	0.762

Consider the returns to scale listed in Table 3, several projects with low carbon emission reduction performance are analyzed. Beijing Gaojing Thermal Power Plant project of Datang Group with the lowest comprehensive efficiency is irs, that is, the proportion of input increase is less than the proportion of output increase, indicating that the project has insufficient input. Huaneng Beijing Gaobeidian Power Plant project, Taiwan Cement project and Conch Group-Baimashan Cement Plant project also have the problem of insufficient investment for increasing returns to scale, which may reflect the incomplete commercialization or financial constraints of these projects. Oxygen-enriched combustion and huazhong university of science and technology of 35 mw project and CRC haifeng carbon capture test project is formed due to scale (DRS) diminishing returns of DEA is invalid, the proportion of the investment increase is greater than the output increase, the proportion of output and input redundancy problem, can according to the actual situation to reduce the money or to strengthen the cost management for the project.

In summary, DEA invalidation is mostly caused by increasing returns to scale in 17 decision making units, indicating that there is a general problem of insufficient investment in all CCUS demonstration projects in China at present, which is related to the financing mode of carbon capture technology development in China at the present stage. When evaluating the economic benefits of Carbon capture projects in China, Liu Muxin mentioned that the business model of CCUS projects in China is unreasonable and there are certain financing difficulties. CCUS projects in China are mostly funded by enterprises themselves. Due to unstable project income and high technical risk, the fund raising is insufficient, which further affects the project scale.

CONCLUSIONS AND RECOMMENDATIONS

China is a major emitter of CO₂, and the carbon neutrality goal defines the basic positioning of CCUS in China's low-carbon development strategy. As a key technology to achieve the carbon neutrality goal by 2060, it is very important and necessary to explore the development status and improvement path of carbon capture, utilization and storage technology. In this paper, DEA data envelopment model is used to select input and output indicators that can reflect emission reduction efficiency and economic benefit, and empirical analysis is carried out on 17 domestic carbon capture utilization and storage demonstration projects that can generate industrial income, and the comprehensive efficiency value of the empirical results is further decomposed. This paper analyzes the reasons for the low carbon emission reduction performance of DEA ineffective projects from the perspective of pure technology and project scale, and puts forward the corresponding improvement path.

China's carbon capture, utilization and storage technology overall carbon reduction efficiency is not high. economic benefits are not obvious: Industrialization development is insufficient, resource allocation needs to be further improved; Low scale efficiency cannot transform mature low-carbon technology into ideal output level; The scale of some projects does not match the input and output, and there are problems of insufficient financing and poor management. According to the research results of this paper, the future development of CCUS in China can be improved from the following aspects:

(1)Adjust the level of resource allocation and pay attention to economies of scale.

(2)Continue to promote CCUS technology emission reduction and provide preferential policies.

(3)Accelerate the industrialization of CCUS technology and improve the project income level.

(4)Learn from foreign advanced experience and strengthen the construction of the whole CCUS process.

REFERENCES

- Charnes A, Cooper W W, Rhodes E. Measuring the efficiency of decision making units[J]. European journal of operational research,1978,2(6): 429-444.
- Du Kerui, ZOU Chuyuan. Regional differences, influencing factors and convergence of carbon emission efficiency in China: An empirical study based on stochastic frontier model and panel unit root [J]. Zhejiang Social Sciences,2011(11):32-43+156.]

- Jose L. Zofio, Angel M. Prieto. Measuring Productive Efficiency in Input-Output Models by Means of Data Envelopment Analysis [J]. International Review of Applied Economics, 2007, 21(4).
- Li Xiaochun, Zhang Jiutian, Li Qi, Liu Guizhen, Zhang Xian, Wei Feng. Evaluation and analysis of implementation of China's Carbon capture, utilization and storage Technology Roadmap (2011 edition) [J]. Journal of science and technology,2018,36(04):85-95.
- Liu Muxin, Liang Xi, Lin Qianguo. Economic benefit and risk assessment of carbon capture, utilization and storage projects in China in the context of carbon neutrality [J]. Thermal power generation: 1-9 [2021-05-10]. https://doi.org/10.19666/j.rlfd.202101009.
- Lozano S, Gutiérrez E.Non-parametric frontier approach to modelling the relationships among population, GDP, energy consumption and CO2 emissions[J]. Ecological Economics, 2008, 66(4): 687-699.
- Maciel C.Environmental efficiency and regulatory standards: The case of CO2 emission from OECD industries[J]. Resource & Energy Economics,2001, 23(1):63-83.
- Szabolcs Fogarasi, Calin-Cristian Cormos. Assessment of coal and sawdust co-firing power generation under oxycombustion conditions with carbon capture and storage[J]. Journal of Cleaner Production, 2017, 142.
- Sun Liang, Chen Wenying. Impact of carbon tax on CCUS source-sink matching: Finding from the improved ChinaCCS DSS[J]. Journal of Cleaner Production, 2022, 333.
- Wang Yan, Su Yi. The influence factors of China's energy saving and emission reduction efficiency from the perspective of green development: An empirical study based on super-efficiency DEA and Tobit model [J]. Management review,2020,32(10):59-71.]
- Ye Yao, Yan Xia, Ying Fan, Maorong Jiang. Research on the path of China's 2030 regional emission reduction target based on environmental production technology efficiency [J]. Resources science, 2017, 39(12): 2335-2343.
- Yu Biying, Zhao Guangpu, AN Runying, Chen Jingming, TAN Jinxiao, Li Xiaoyi. Journal of Beijing University of Technology (Social Science Edition), 201,23(02):17-24.
- Zhang Qingyu, LIAO Mingqiu, Han Yongming. Computer and applied chemistry, 2016,33 (5) : 615-622.]