Inorganic Element Functional Group Database on Pulverized Coal Surface Based on XPS Method

Hu Yi , Li Peisheng
College of Power & Mechanical Engi.,
Wuhan University,
Hubei,China,
huyi1982115@sohu.com

1.Abstract

The studying achievements of coal characterization using XPS method are summarized. Microsoft Visual Studio. net is utilized to build functional group characterization database of coal , including the kind of functional groups, binding energy values, coal species, producing areas, sample preparations and literature informations etc. It can be used to search and analyze data of XPS on coal conveniently, and is also of significance for further coal study with XPS method.

2.Introduction

1. What is XPS ?
2. The development of applying XPS to coal.
3. The existing problems .
4. Measurement ——building an XPS database of coal

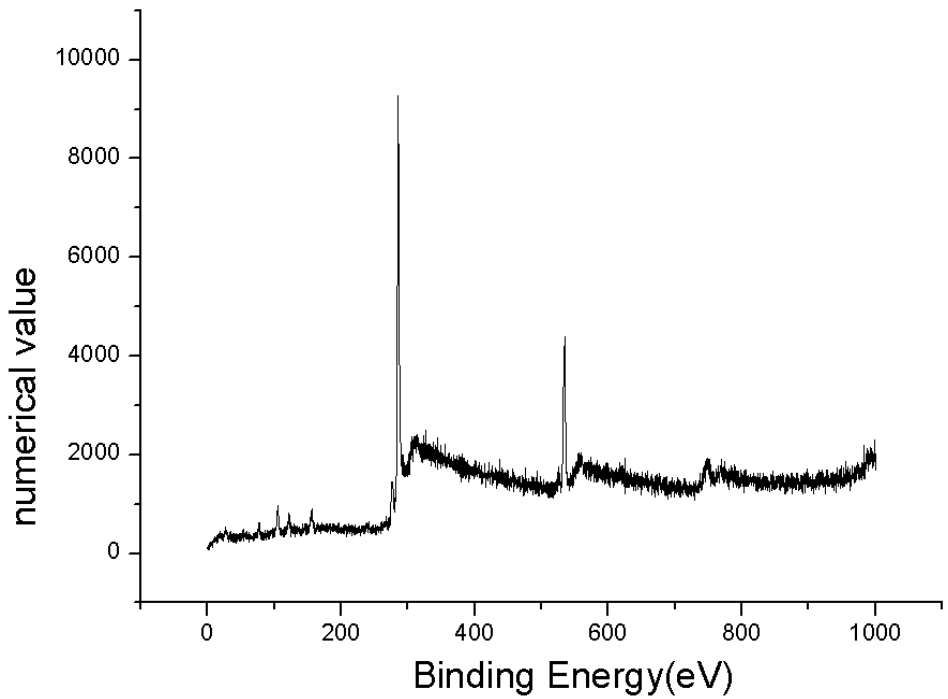


Figure 1. XPS spectral line of one coal.

X-ray photoelectron spectroscopy (also known as ESCA) is a kind of method for solid materials surface analysis. It can determine the elemental composition of surfaces, as well as distinguish between the different chemical environments of a given element. It is widely utilized in the domains of coatings, sensors, catalysts, biomaterials, electronic materials etc. and was firstly used on coal in 1974.

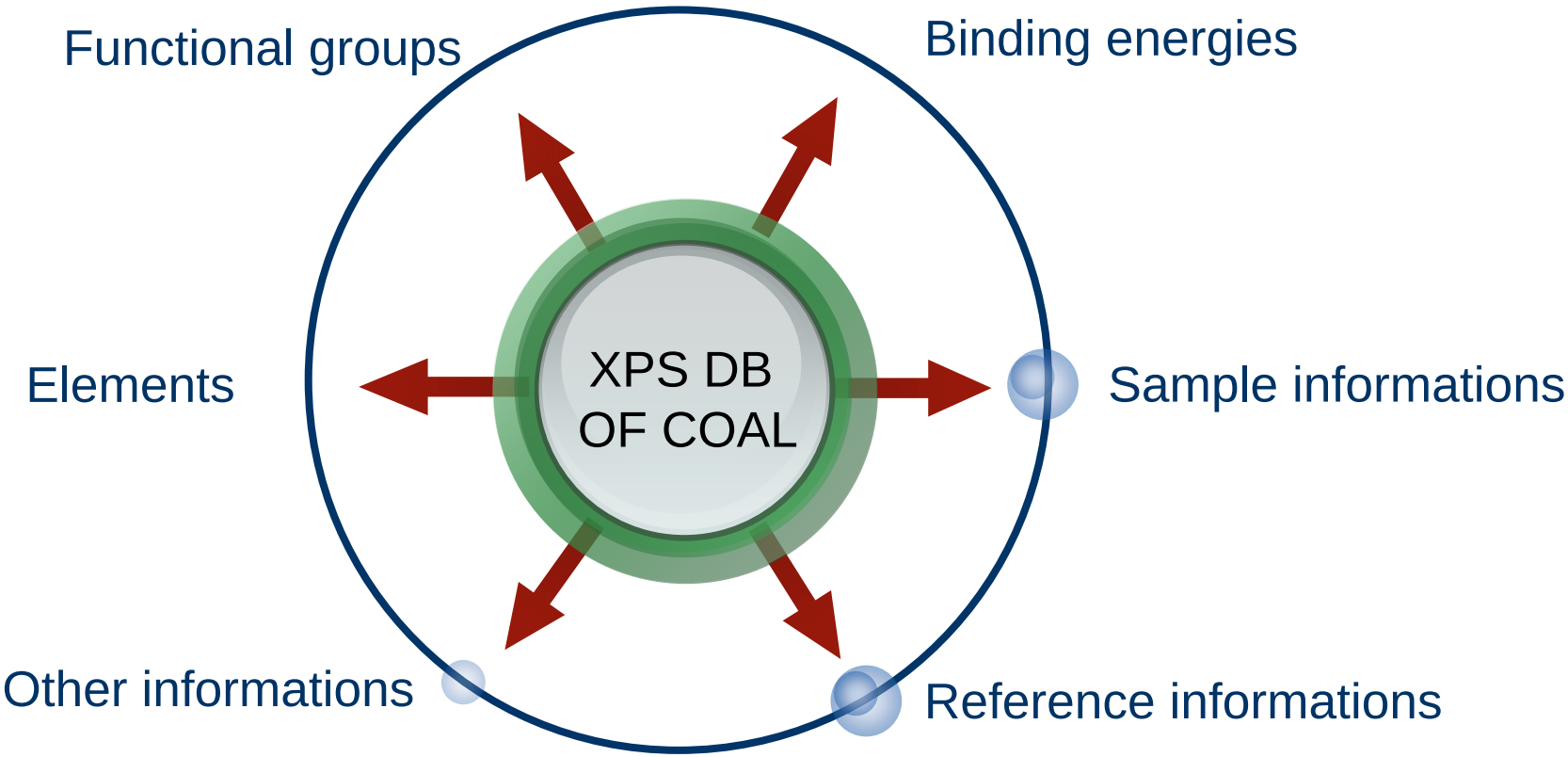
- Frost analyzed the existing states of C, O, S in several coking coals
- Brown examined a number of coals and their ashes concluding carbon exist as graphite ,hydrocarbon, carbonyl, carboxyl.
- Wallacc studied the existing states of nitrogen in coal concluding that organic nitrogen is main in pyrrole and pyridine.
- Perry find XPS spectral line of sulfur in coal can be resolved into two components, corresponding to organic sulfur and sulfate.
- Chen peng, Liu yanhua etc. studied typical coal in China using XPS method.

Coal is a complex compound containing a lot of functional groups of C,O,N,S, whose binding energies may be close to each other , even overlap.

Differences in experimental apparatuses and energy calibrations for different persons.

Differences in coal species, producing areas and sample preparations.

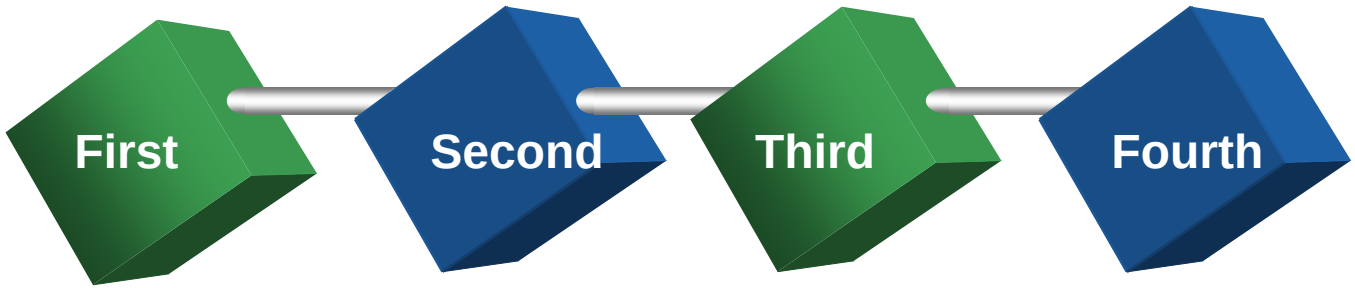
Small deviation of elementary binding energy—inducing the problems of identifying sub-peaks and their binding energies and further studying of quantification.


Functional groups
Binding energies
Elements
XPS DB
OF COAL
Sample informations
Other informations
Reference informations

3.Discussing

1. Data compilation

2. GUI design, search strategy and implementation



First	Second	Third	Fourth
Literature search of published papers	Review papers and select the ones having adequate informations	Checks for consistency; classify and enter the data into database	Data verification

GUI design, search strategy and implementation

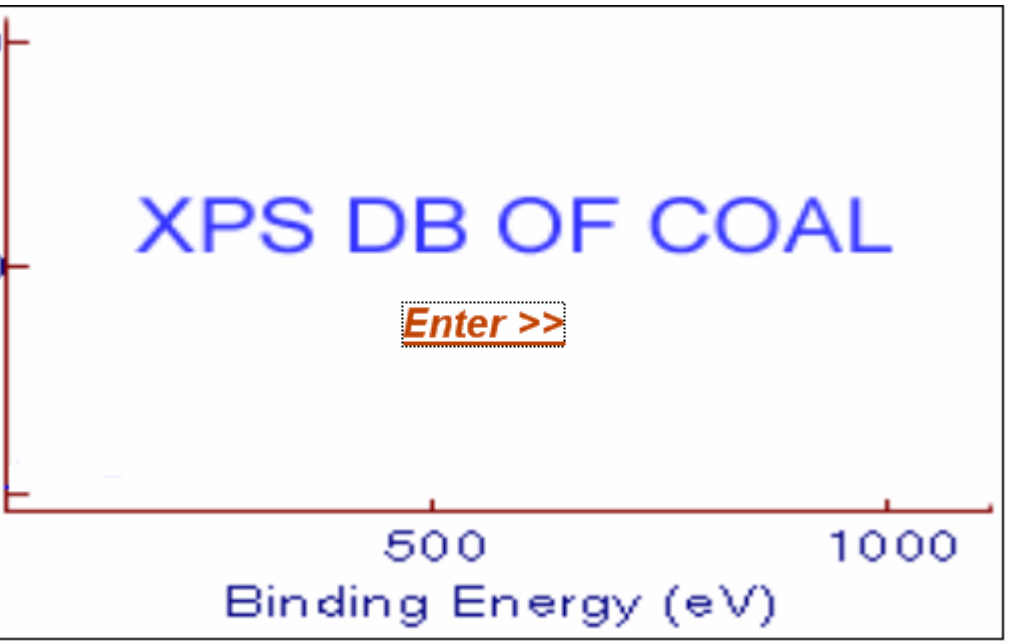


Figure 2.Start-up interface of XPS DB of coal

Two search strategies

1.Identify binding energy and functional group by elementary spectral line.

2.Identify functional group and unknown spectral line by binding energy .

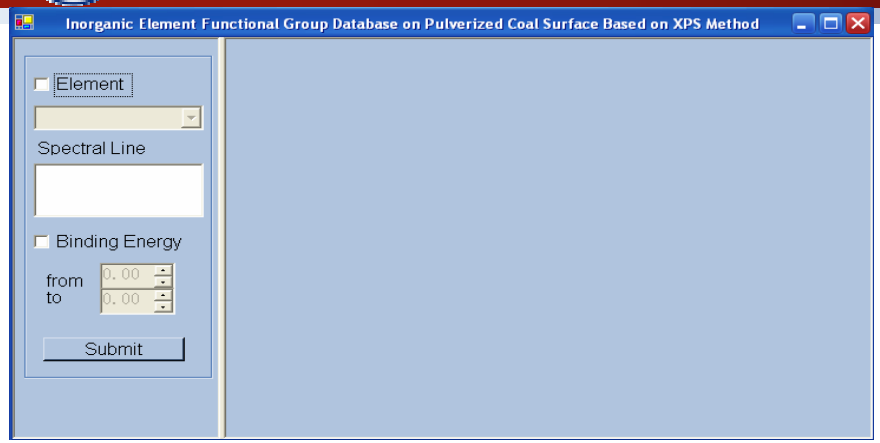


Figure 3.GUI for searching

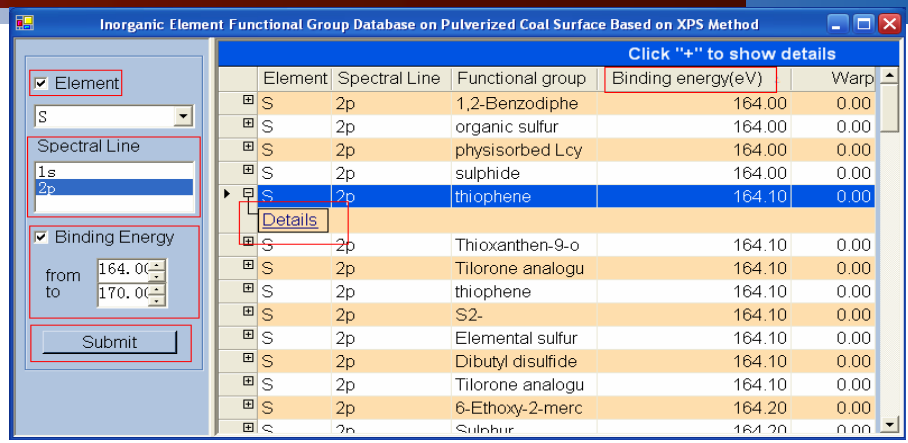


Figure 4.GUI of identifying binding energy and functional group

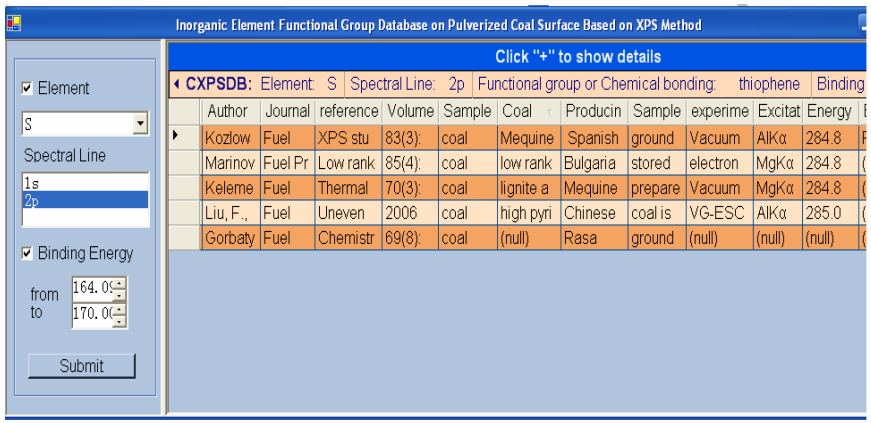


Figure 5.GUI of detail informations

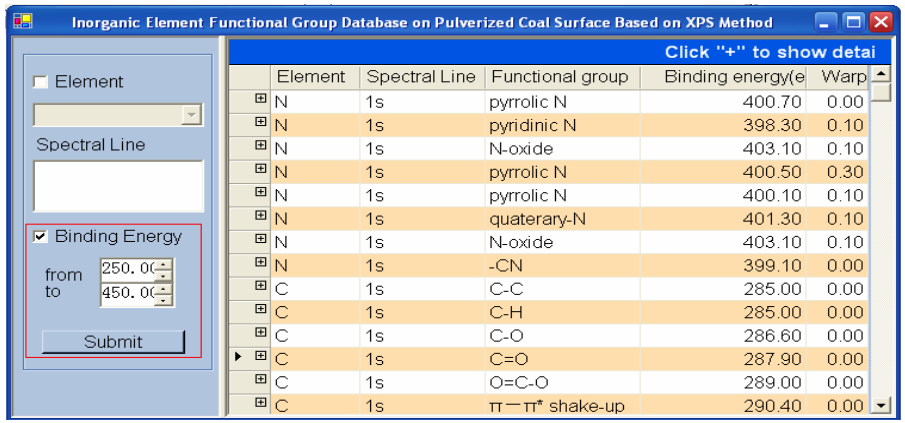


Figure 6.GUI of identifying functional group and unknown spectral line

4.Application

Photoelectron spectra is obtained using XSAM800 ESCA spectrometer equipped with MgKα excitation source ,which is made by KRATOS company. The analysis mode of FRR is used ; The pressure in the analysis chamber is lower than 5×10^{-7}Pa . Calibration is carried out to the main C 1s peak at 284.6 eV.

Table1 .Proximate and Ultimate analysis of coal sample

NO.	Proximate analysis (WT %)				Ultimate analysis (WT %)					Qd (MJ.KG^{-1})
	M	V	A	FC	C	H	O	N	S	
Coal sample	1.28	21.76	16.19	60.77	70.68	5.52	4.02	1.68	0.63	33.34

The result is obtained that C in coal mainly present as graphite(284.4±0.3) ; hydrocarbon(285.0±0.3eV); hydroxyl or ether(286.1±0.2eV); carbonyl(287.6±0.3eV); carboxyl or ester(288.6±0.4eV) and π－π* shake up (291.2±0.2eV) by Identifying binding energy and functional group by elementary spectral line in XPS DB OF COAL . The C1s spectral line and the result of peak-spliting of the coal is shown in figure 7. The data of sub-peaks can be used to further analysis. Of course ,the functional groups of O,N,S can be obtained by the similar way.

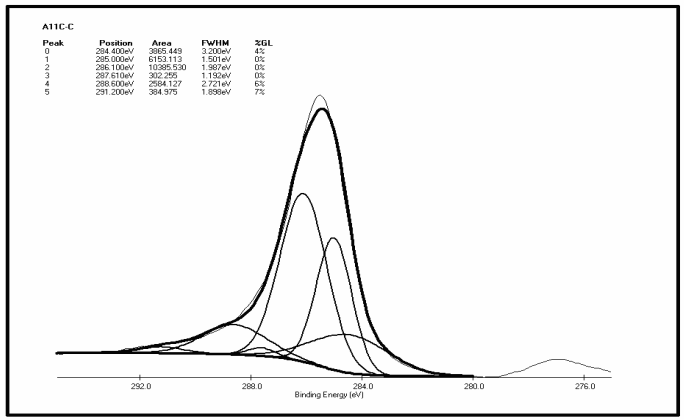


Figure 7. C1s spectral line of one coal

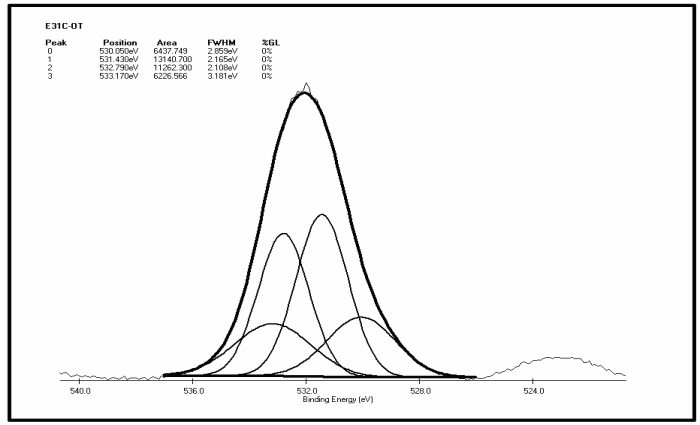


Figure 8. O1s spectral line of one coal

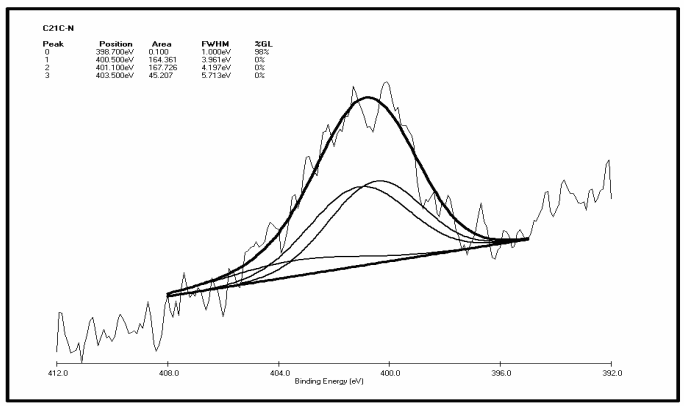


Figure 9. N1s spectral line of one coal

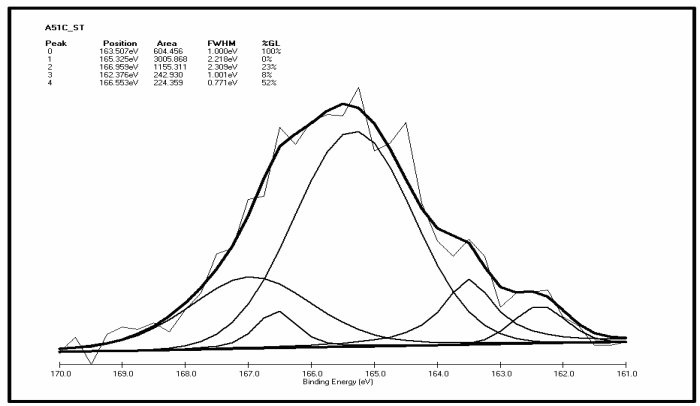


Figure 10. S2p spectral line of one coal

5.Conclusion

1. The building and application of this XPS DB is of significance for searching experimental data conveniently and exactly.

2. Web-based database is planned to be built .

3. This database will be refreshed with development of XPS study of coal .

THANK YOU !