

*Share your Material Studio project dir with Vasp Studio is highly recommended.

***Ctrl + S to save anytime!**

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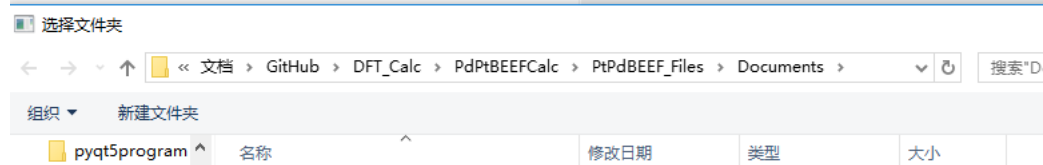
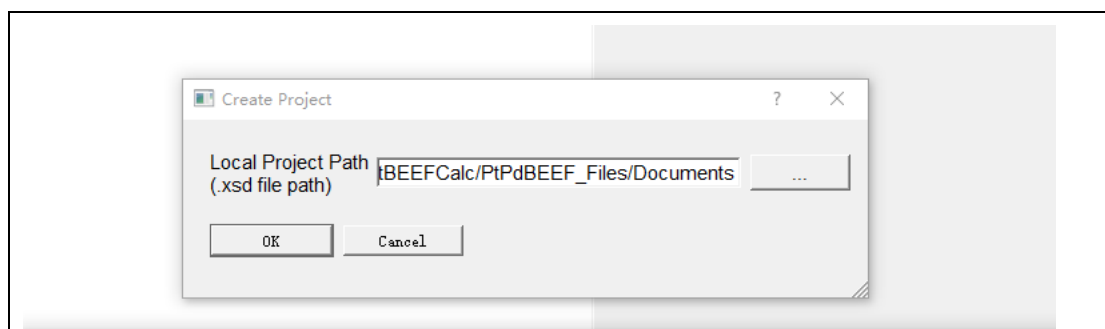
Notice

1. Only support ssh login to submit job on Linux.
2. Only support trans your xsd file from Material Studio, and submit job with VASP.
3. If you met problems, just submit issues on Github project page, or fix it and submit through fork-pull request process

How To Submit Jobs?

1.Create or Open a Project.

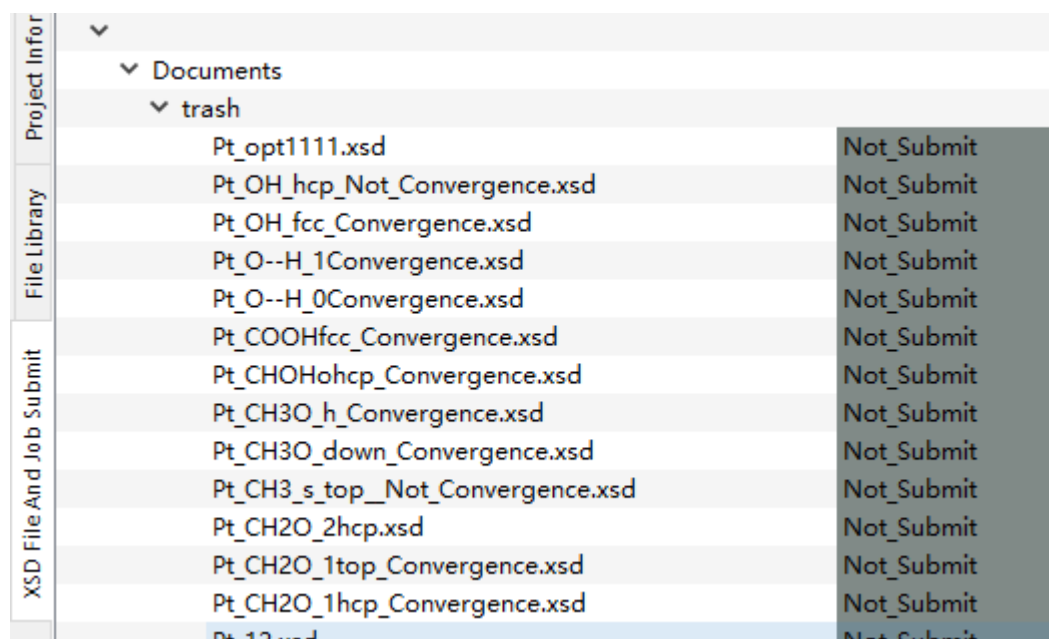
Project-NewProject, choose a dir contains .xsd files, Material Studio's Documents dir is recommended.



Then give a path to save .vsp file, open project with this file later.

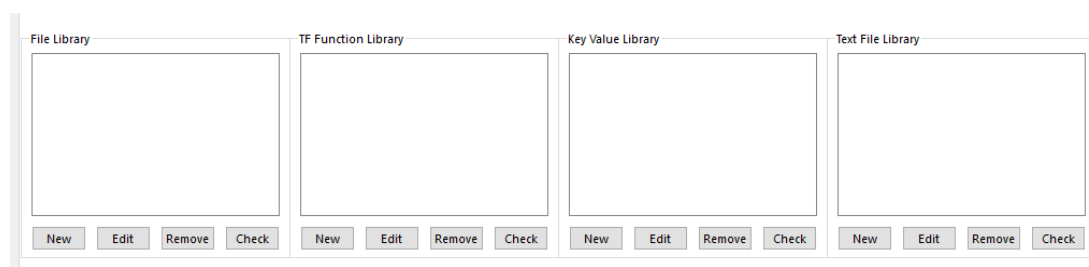
Open Project: Project-OpenProject, choose a .vsp file

After creating your project, VS will search all .xsd files, and make them a tree.



Attention, for compatible with linux, your .xsd file name should contain only alphabet, numbers and - _ symbol.

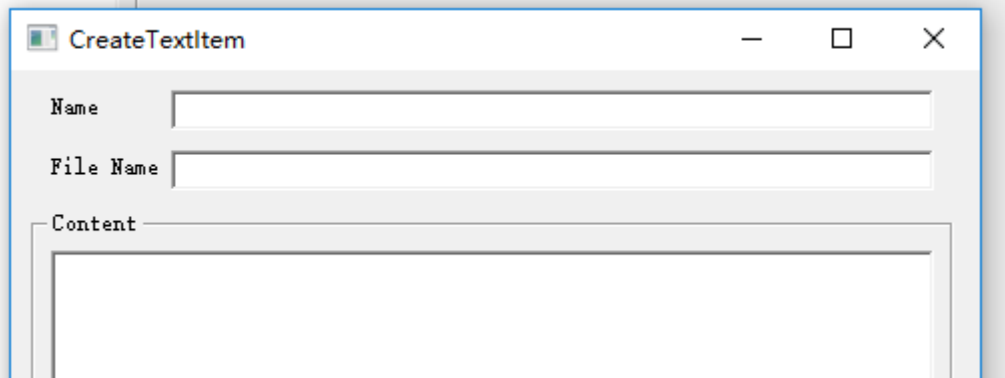
2.Preapre for Creating Lib Files.



There are 4 types of lib files: Text File Lib, File Lib, TF Function Lib and Key Value Lib.

- Text File lib is used to store text file like INCAR, POSCAR. POSCAR and fort.188 file (if you need) have a template (used to help store position from .xsd file), I'll give them later. When you submit jobs, VS will create a text file, its name and content is what you set in lib, these file will copy to each VASP dir, but POSCAR and POTCAR changes according to your .xsd files.
- If what you submit job need is not a text file or not recommended as a text file (like a binary file of linux .sh file), then you need create a File Lib, just give the file path. When you submit jobs, these file will be copied to each VASP dirs.
- There is a T T T and F F F to define if your atoms allow to move in POSCAR, this is done by setting a python function, details later.
- Key Value Lib is used to set some parameters which is not suitable for VS to add it in UI, details later.

The window of creating libs is like:

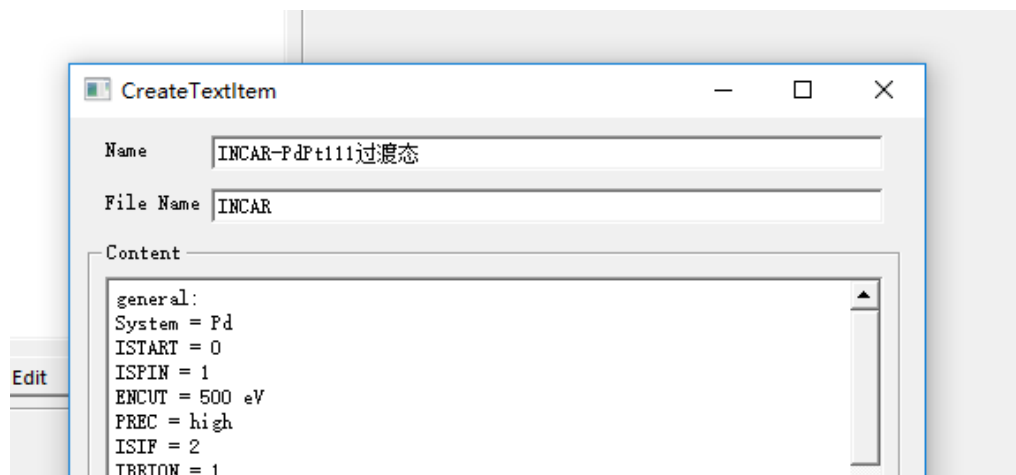


Every lib creating window contains a **Name**, which is the **Key** for VS to include these lib files, so these Names should be **Unique**.

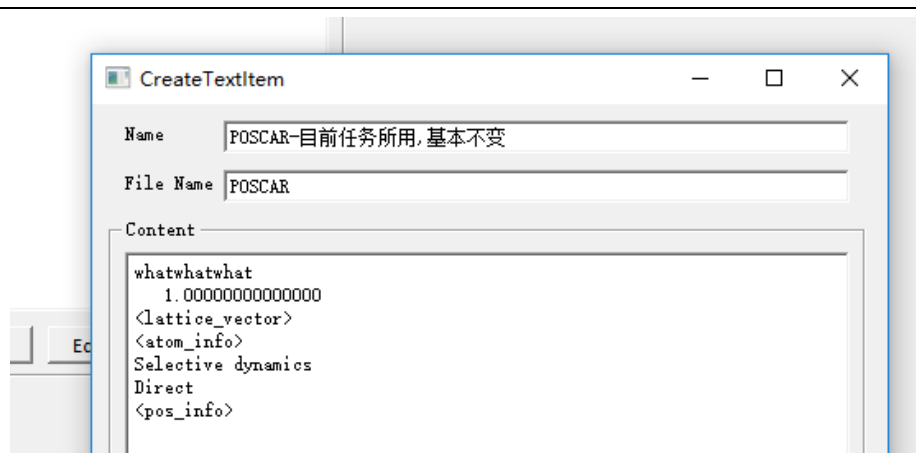
Check button in the window is invalid now.

3.Create Text File lib

When you submit job, VS will create a text file in each VASP dir, this file's name is **File Name**, and its content is **Content**. You can create many INCAR or KPOINTS for what you need in different tasks.



POSCAR template:



whatwhatwhat

1.000000000000000

<lattice_vector>

<atom_info>

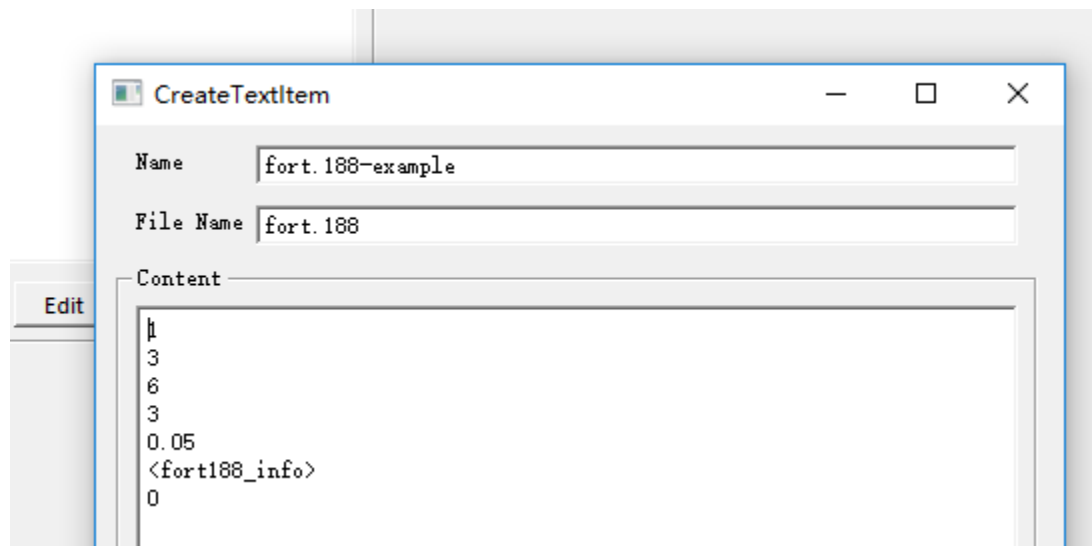
Selective dynamics

Direct

<pos_info>

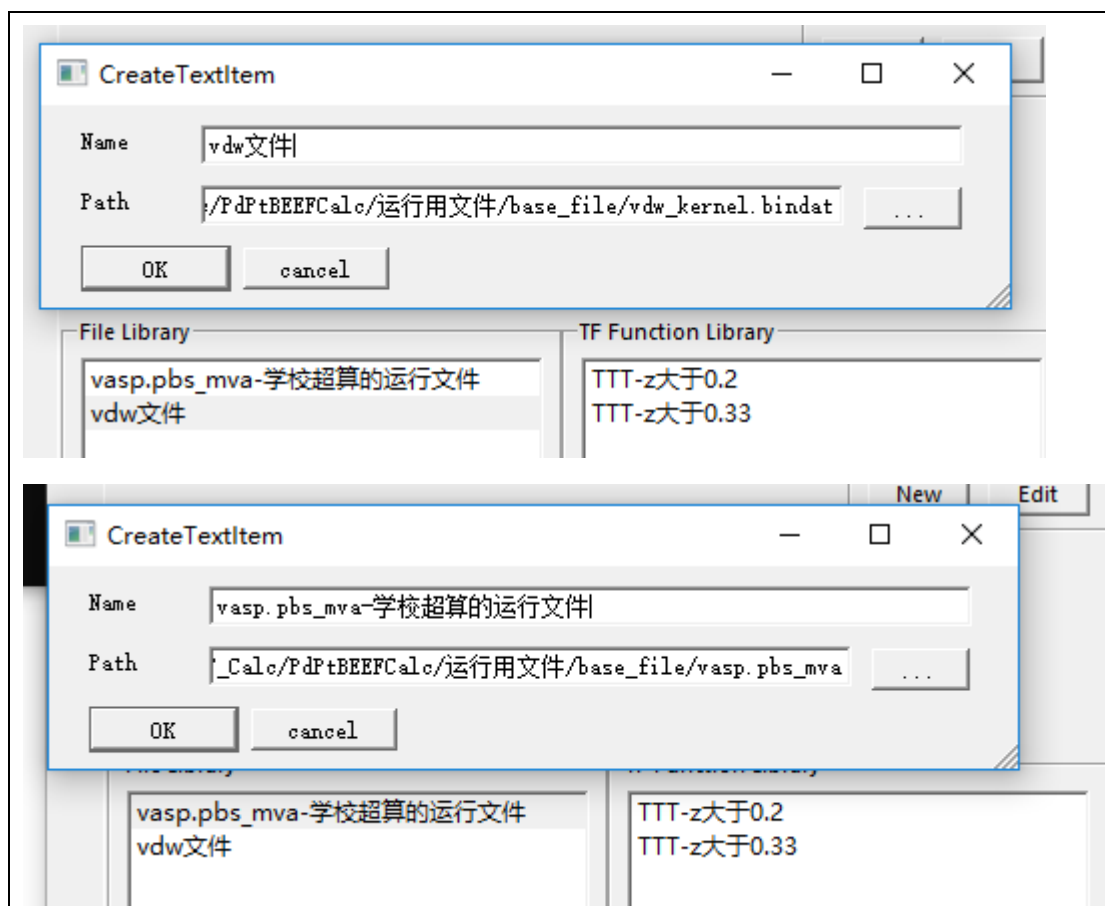
Remember to keep <pos_info> ..., these are placeholders for the information extract from .xsd file.

If you use fort.188, the templates is:



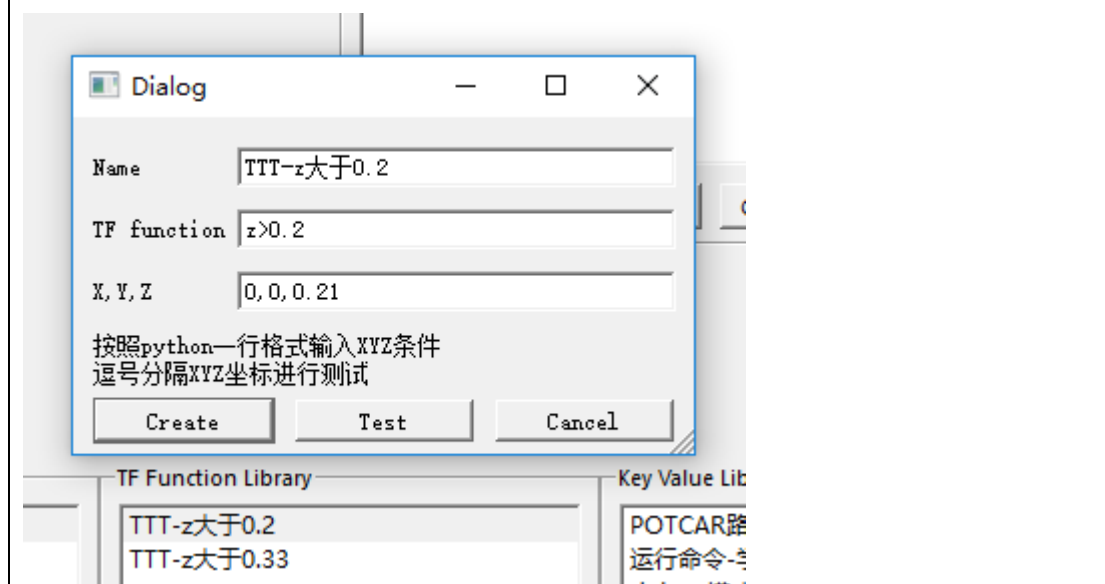
4.Create File Lib

Just set Name and the path.



5.Create TF Function Lib

Judge TTT of FFF in your POSCAR, set TF function in **Python** style, input parameters are ONLY **x, y, z**, e.g.



Also you can set: $x > 0.5$ or $y < 0.1$ or $z > 2$, then you can put your coordinates in X, Y, Z, number divided by comma, push **Test** to give results and push **Create** to check if it is valid and create.

6.Create Key Value Lib

KeyValue Lib stored some configuration which is not very common, for VASP jobs, you **Have To** create:

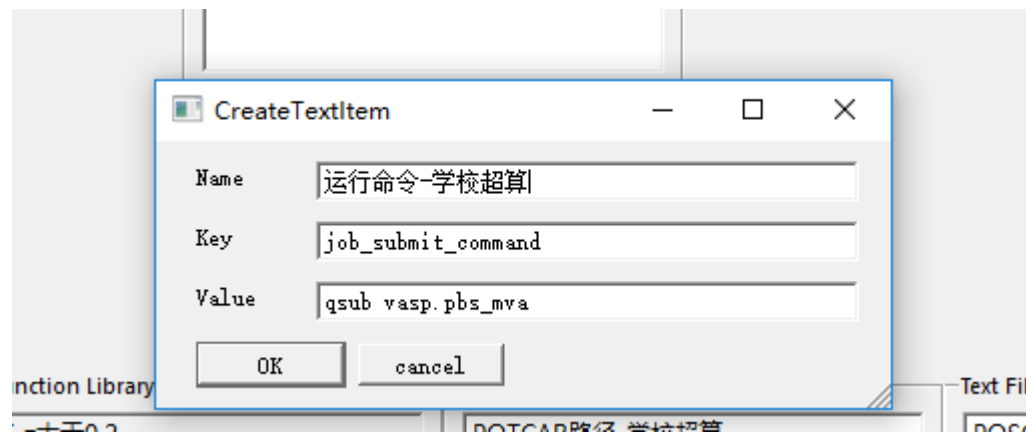
1. remote_base_POTCAR_dir:

put the string **remote base POTCAR dir** in **Key** and set POTCAR path



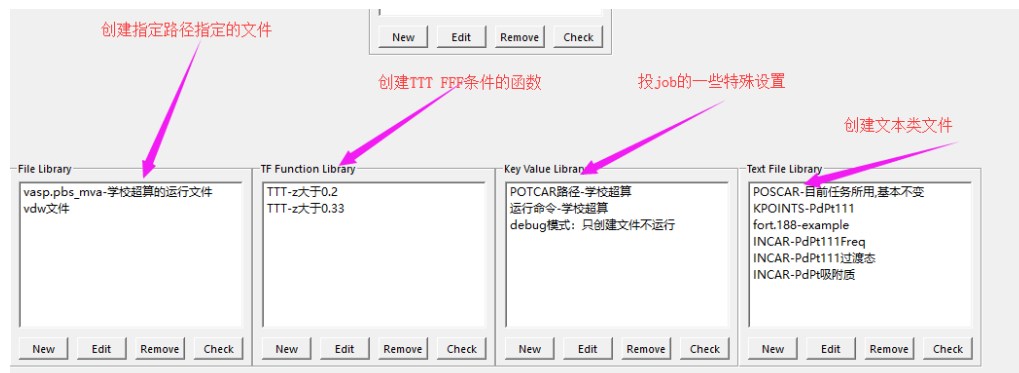
2. job_submit_command, set job submit command, like sh <name>.sh

or qsub <script_name>

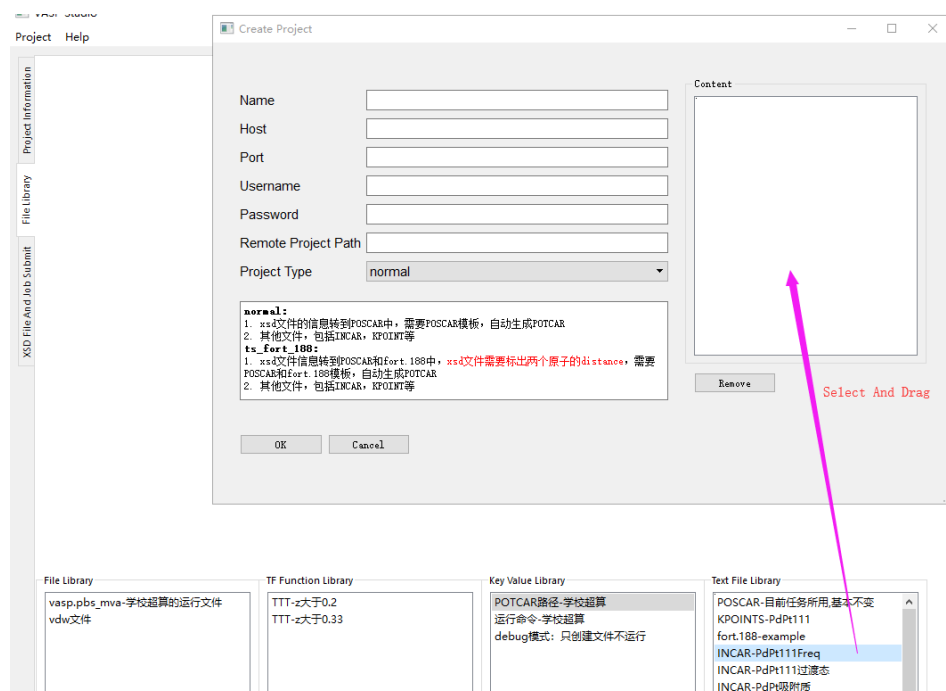


7.Create a Job Submit Configuration

This is an example of my libs:



This lib file can be seen as basis, you need to add these basis when you are creating your submit job config. Push **New** button in Job Submit, and **Just Drag And Drop to Content**.



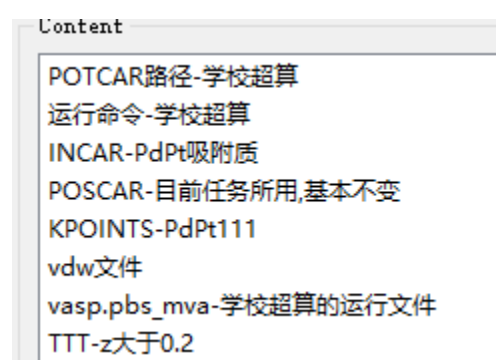
Other paramters, like Host, Port, Username and Password are essential for login ssh. Remote Project Path is the path to store your VASP dir, **it's high recommended to give an individual dir for differe tasks, like**

vsJob/TS or vsJob/Freq.

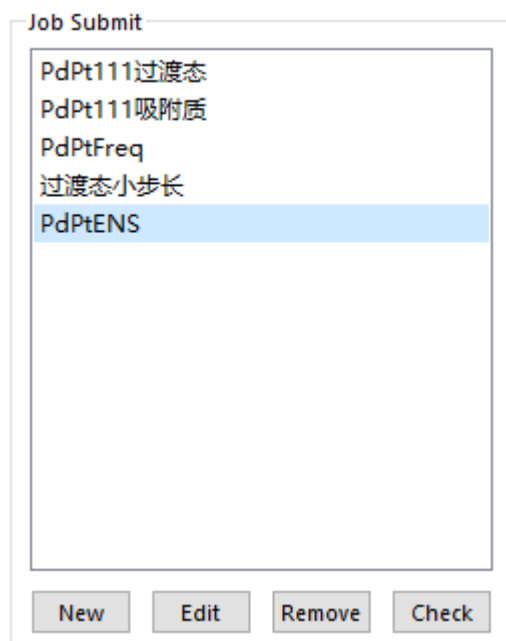
Project Type

If you use fort.188 to calculate transitions state, change **Project Type**, otherwise, keep normal.

Different tasks needs different **Content**.

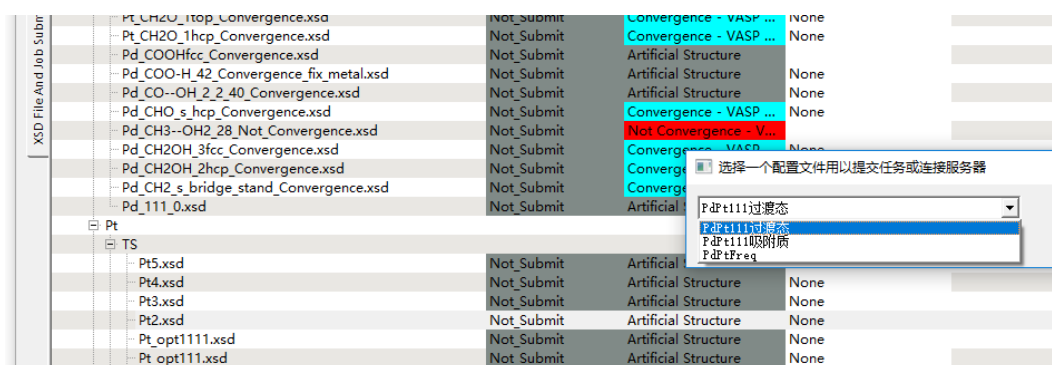


Create Job Configuration from different combination of Libs.



8.Work Area and Job Status

Click and trigger **Submit Job**, then choose one of the job configuration, then click OK, click OK...



If you submit your job successfully, WorkNode will record your job node.

	149265.node1
0.04913	146618.node1
	146665.node1
0.04774	146505.node1
	146666.node1
0.04800	146506.node1

***WorkNode** is on the right side of header, you need to drag left.

Type	Mark	Energy	Final RMS	Work Node	Job	Match State
Convergence - VASP ...	None			160821.no...	PdPtENS	None

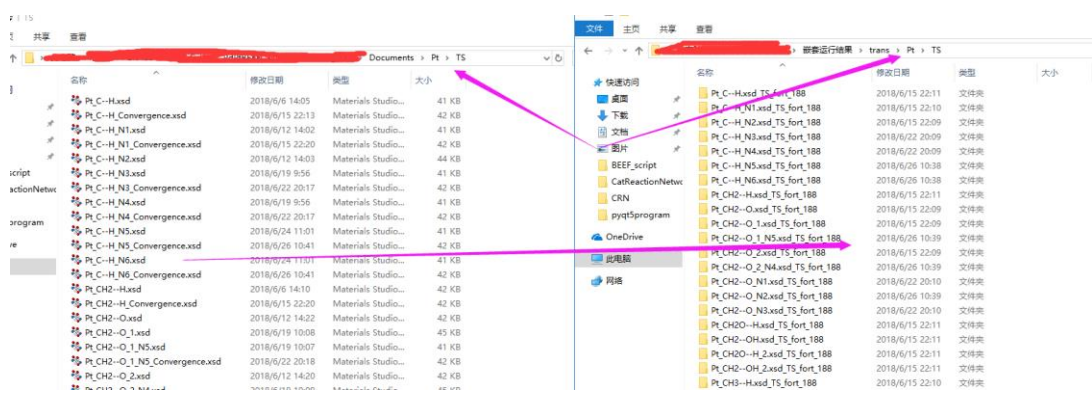
How To Manage Your Job?

1.Link with VASP dirs.

To extract frequency, energies and RMS, you need to link these jobs to VASP dir. Until now, VS only supports for downloading VASP dirs from

HPC or server and link locally. (VASP Studio v0.2)

Remember only download the dirs you set in the *remote_project_path* or add VASP dirs into the existing dirs which has a same structure as your *remote_project_path*. E.g. I set a remote project path like vsJob/freq, there are files like vsJob/freq/Pt/CH and vsJob/freq/Cu/CO, I just download the whole vsJob/freq dir to a certain local dir, or download vsJob/freq/Ni/CO into existing local dirs.



That's because VS link the job with VASP dir **By Path**, **By Path** means job links only when there is a VASP dir path complete same as .xsd file path. E.g. I have made a project at C:/wang/, I have C:/wang/Pd/111, I download Pd/111 from HPC to C:/results, so when I use **Local Link – By Path**, I will choose the dir C:/results.

Another way to link files is to use **By Name**, if your .xsd file name is same with the VASP dir, then it links. (If there are two VASP dir mathes, only the first VASP dir will link)

Pt_H-CHO_Convergence.xsd	Freq_Check_Fail	Convergence - \
Pt_H-CHO_0Convergence.xsd	Submitted	Convergence - \
Pt_H-CHO.xsd	Convergence	Artificial Structur
Pt_H--CH2OH_N1_Convergence.xsd	Freq_Check_Pass	Convergence - \
Pt_H--CH2OH_N1_0Convergence.xsd		Convergence - \
Pt_H--CH2OH_N1.xsd		Artificial Structur
Pt_H--CH2OH_Convergence.xsd		Convergence - \
Pt_H--CH2OH.xsd		Artificial Structur
Pt_H--CH2O_4.xsd		Artificial Structur
Pt_H--CH2O_3_Convergence.xsd		ence - \
Pt_H--CH2O_3.xsd		Structur
Pt_H--CH2O_2_Convergence.xsd		Convergence - \
Pt_H--CH2O_2.xsd		Artificial Structur
Pt_H--CH2O.xsd	Not_Convergence	Artificial Structur
Pt_CO--H_N1.xsd	Submitted	Artificial Structur

After Linking, the status will turn:

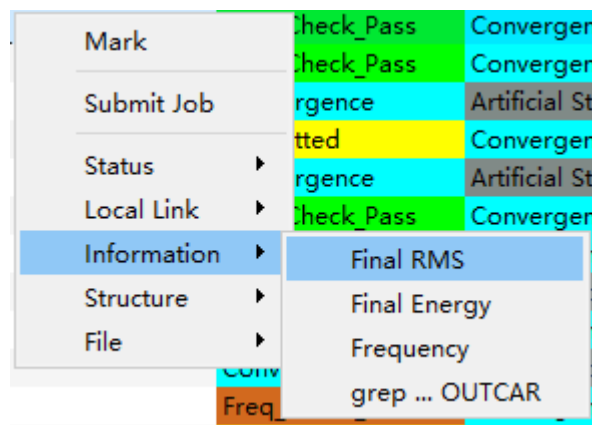
Pd_CO--O_3_39_Convergence.xsd	Freq_Check_Pass
Pd_CO--O_3_39.xsd	Finished_And_Linked

And you can see local_vasp_dir

Match State	submit_job
40/40	None
None	local_vasp_dir
40/40	C:/Users/wang/Desktop/运行结果/PdPt/Trans/Pd_CO--
None	H_2_36.xsd
None	energy
42/42	-75.52907546
None	final_RMS
42/42	0.04776
None	status
41/41	Convergence
None	node1
None	None
41/41	RMS_array
41/41	[9.22577 3.402625 2.672418 1.506582 1.624839
None	1.538977 1.608241 1.60049 1.605023 1.48716 1.679707
40/40	1.605857 1.635767 1.543055 1.692345 1.606243
None	1.559212 1.577216 1.59837 1.864123 1.788493 1.72908
40/40	1.546752 1.577258 1.543795 1.595025 1.681746
40/40	1.691829 1.513386 1.677089 1.682785 1.71486
None	1.509171 1.638177 1.667782 1.578501 1.705071
39/39	1.71099 1.578838 1.596421 1.666546 1.726072
None	1.509589 1.628675 1.660586 1.835065 1.681786
None	1.768173 1.744815 1.704875 1.556155 1.687256
39/39	1.671395 1.72863 1.530025 1.715776 1.591006
None	1.480324 1.619744 1.60855 1.580527 1.57314 1.640447
39/39	1.560066 1.594244 1.637002 1.677088 1.7264 1.907673
None	1.694282 1.680459 1.576208 1.446227 1.533758
39/39	1.416869 1.418625 1.550014 1.569683 1.733522
39/39	
None	

2.Information Extract and Final Structure Export

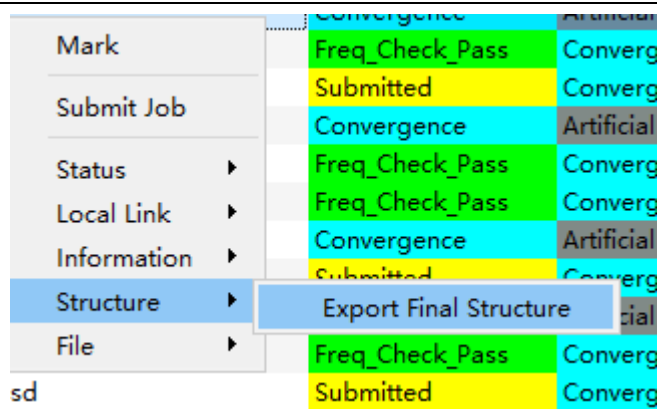
You can get information and final structure then, choose the jobs and right click on Final RMS, Final Energy or Structure-Export Final Structure.



If you submit a job to calculate frequency, extract Frequency, then you need to give a **Right Imaginary Frequency Count**, normally 0 for Intermediates and 1 for transition states.

Not_Submit	Not Convergence - V...	
Convergence	Artificial Structure	
Freq_Check_Pass	Convergence - VASP ...	
Freq_Check_Fail	Convergence - VASP ...	None
Freq_Check_Fail	Convergence - VASP ...	None
Submitted	Convergence - VASP ...	
Not_Submit	Not Convergence - V...	
Not_Submit	Not Convergence - V...	

Structure-Export Final Structure to export final structure.

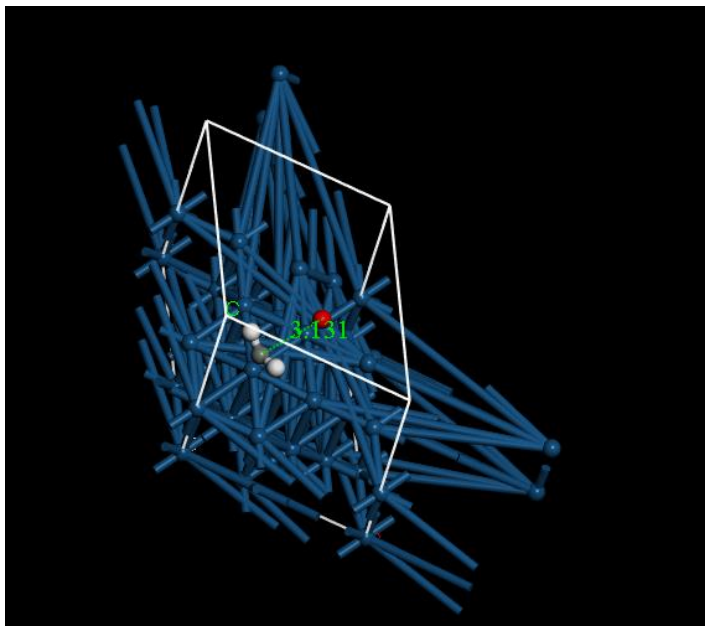


Exported xsd file add _NotConvergence or _Convergence to the original name, **it is highly recommended to keep the name unchanged.**

Match State needs to be larger than 1, then exported structure will be valid.

rk Node	Job	Match State
950.no...	PdPtFreq	None
		43/42
		None
		None
375.no...	PdPtFreq	None
374.no...	PdPt111吸...	None
373.no...	PdPt111吸...	None
		42/41
		42/41
		42/41
		42/41
		None
		None
377.no...	PdPt111吸...	None
		41/40

Sometimes you met such bug:

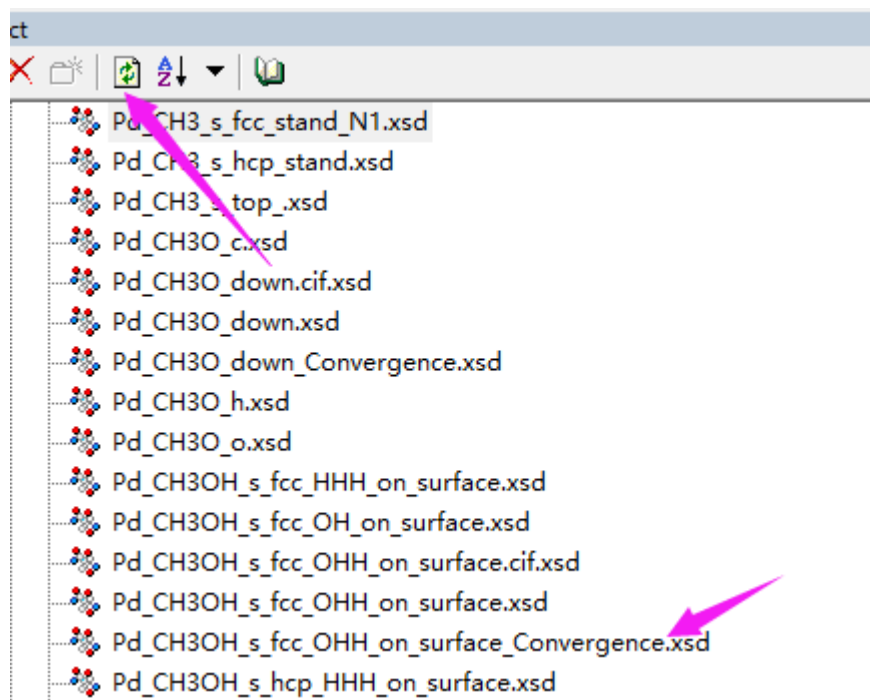


Just delete bonds and Monitor bonding.

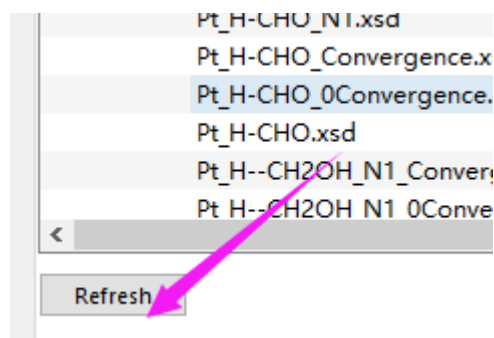
Exported .xsd file can submit other job, often you submit frequency job after a Convergence Structure.

3.VS with Material Studio

Just click **Refresh** on Material Studio, then exported structure will show.



You can export NotConvergence Structure, **Rename** and **delete** “_NotConvergence”, then click **Refresh** on VS, the new file will show.



4. Mark

Anytime you can choose jobs and right click trigger **Mark**, choose a color and make notes to your jobs.

Pt_UO_s_bridge.xsd	Convergence	Artificial Structure	完成	-114.623474
Pt_CHOHplane2.xsd	Convergence	Artificial Structure	完成	-121.472790
Pt_CHOHplane1_Convergence.xsd	Freq_Check_Pass	Convergence - VASP ...	完成	
Pt_CHOHplane1.xsd	Convergence	Artificial Structure	完成	-121.470597
Pt_CHOHplane1.cif.xsd	Convergence	Artificial Structure	完成	-121.470597
Pt_CHOHohcp.xsd	Convergence	Artificial Structure	完成	-120.920406
Pt_CHOHofcc.xsd	Convergence	Artificial Structure	完成	-120.910442
Pt_CHOHchcp.xsd	Convergence	Artificial Structure	完成	-121.470105
Pt_CHOHcfcc.xsd	Convergence	Artificial Structure	完成	-121.466276
Pt_CHOH22.xsd	Convergence	Artificial Structure	完成	-121.277705
Pt_CHO_s_top_Convergence.xsd	Freq_Check_Fail	Convergence - VASP ...	正在投	
Pt_CHO_s_top.xsd	Convergence	Artificial Structure	正在投	-117.806586
Pt_CHO_s_top.cif.xsd	Convergence	Artificial Structure	正在投	-117.806586
Pt_CHO_s_hcp_1.xsd	Submitted	Artificial Structure	正在投	
Pt_CHO_s_hcp.xsd	Convergence	Artificial Structure	正在投	-117.809126
Pt_CHO_s_fcc.xsd	Convergence	Artificial Structure	正在投	-117.525266
Pt_CH3OH_s_hcp_OHH_on_surface_Convergence.xsd	Freq_Check_Pass	Convergence - VASP ...	完成	
Pt_CH3OH_s_hcp_OHH_on_surface.xsd	Convergence	Artificial Structure	完成	-129.148671
Pt_CH3OH_s_hcp_OHH_on_surface.cif.xsd	Convergence	Artificial Structure	完成	-129.148671
Pt_CH3OH_s_hcp_HHH_on_surface.xsd	Convergence	Artificial Structure	完成	-128.988185
Pt_CH3OH_s_fcc_OHH_on_surface_Convergence.xsd	Freq_Check_Fail	Convergence - VASP ...	完成	
Pt_CH3OH_s_fcc_OHH_on_surface.xsd	Convergence	Artificial Structure	完成	-129.164281
Pt_CH3OH_s_fcc_OH_on_surface.xsd	Convergence	Artificial Structure	完成	-129.027902
Pt_CH3OH_s_fcc_HHH_on_surface.xsd	Convergence	Artificial Structure	完成	-128.992551

5.Delete

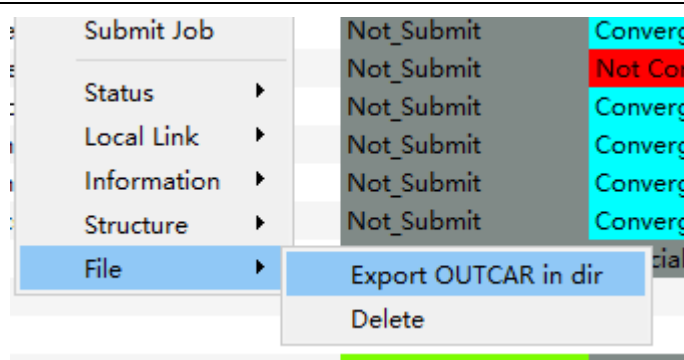
File-Delete, file will be moved to **Trash** Folder under your project dir.

Example

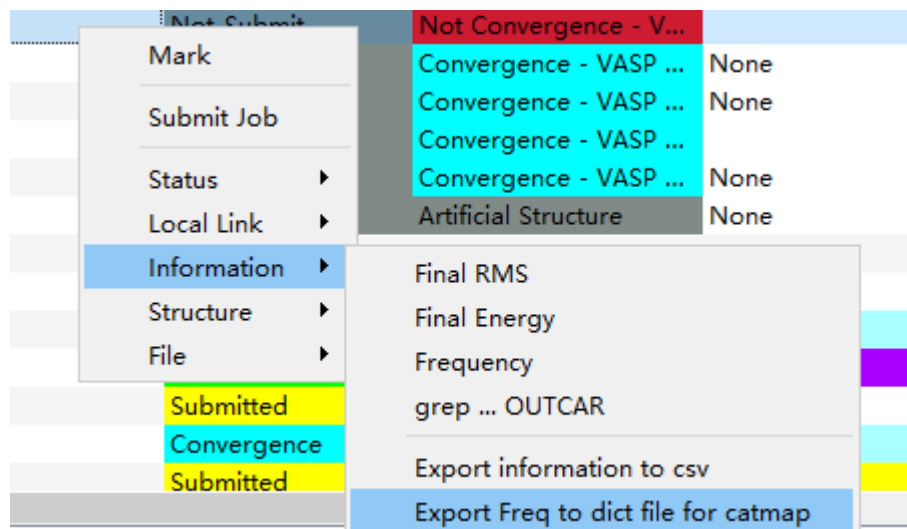
1.Finish preapring BEEF data for CRN

- CRN is another project which have not open-source now.

- 1.Prepare Job Submit configuration for optimization for Intermediate, optimization for Transition states, frequency and BEEF.
2. Get initial structure in Material Studio, submit Transition state and intermediate to get the most stable structure.
3. If has not-convergence structure, modify it and re-submit. If convergence, submit frequency job.
4. If frequency check successfully, mark it with “Finished”, others will need to be modified and submit Optimization again.
5. Mark a blue note if finished, mark a red note if unfinished.
6. Mark all jobs that passed frequency check, export final structure again, and submit BEEF
7. When finished all BEEF jobs and linked, use File-Export OUTCAR in dir to get all BEEF OUTCAR.



9. Use Information-Export Freq to dict file for catmap to export files for Catmap.



10. The BEEF OUTCAR and freq dict is the input for CRN.

Existing Bugs:

1. An 'Enter Key' in KeyValue Library
2. VS crashed when modify Job Submit: that happens when you **RENAMED** your lib, we can only delete that Job Submit and re-create one.
3. Failed to submit fort.188, and there's a KeyError on command line: set Display Style-Lattice to Original in Material Studio, make sure all atoms are on the slab, if there's an atom out of slab, move it back. (Material Studio mark the atom in another periodic box as the image of original atom so I cannot get the corrdiante.)

