



Computational Science
Research Center

KIST-NOMAD

Web Interface for Data Retrieval

Developed by Mr. Samuel Boateng and Chan Soo Kim

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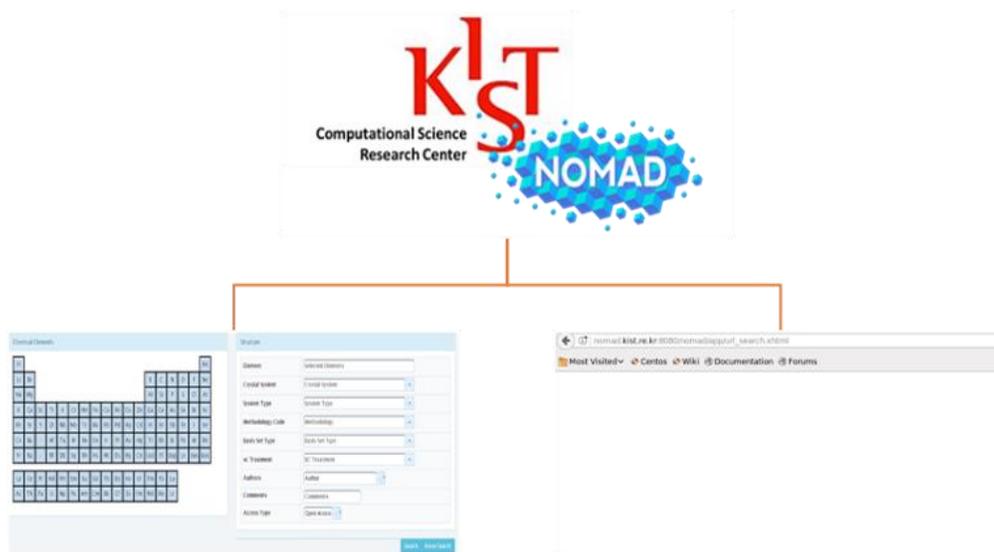
Introduction

The Novel Materials Discovery (NOMAD) Laboratory maintains the largest **Repository** for input and output files of all important computational materials science codes.

The NOMAD Repository, a web based materials data application, was established to host, organize, and share materials data.

KIST Computational Science Center in collaboration with NOMAD EU developed a KIST version of the NOMAD repository. The KIST NOMAD has two components for the retrieval of data.

- i. Interface search
- ii. API based URL search



The URL search is designed for bulk download of calculation files from the KIST NOMAD application.

Application Programming Interface

http://nomad.kist.re.kr:8080/nomad/app/url_search.xhtml

Search Parameters

Search Parameter	Explanation	Search text
Element	Any chemical element/formula. Example H, HCl, TiO ₂ , etc.	element
Calculation method	The method/application used to perform the calculation. Example VASP, Gaussian, Octopus, FHI-aims, etc.	calculation
System type	The system type for the specific calculation. For example 3D, 2D, etc.	system_type
Crystal System type	The crystal system type of the specific calculation. For example rhombohedral, cubic, triclinic, etc.	crystal_type
Basis set type	The basis set type of the specific calculation. For example plane waves, numeric AOS, gaussians, etc.	basis_set_type
Xc treatment type	The XC treatment type of the specific calculation. For example GGA, LDA, hybrid, etc.	xctreatment
Author(s)	The author(s) of the specific calculation. For example Johnson Russel	author

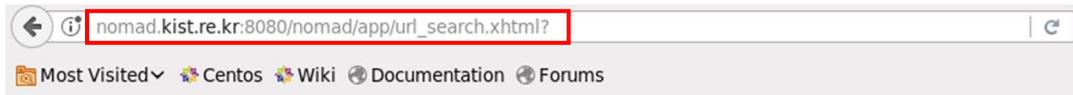
Performing a search

The application allows for searching with a single parameter and a combination of all or a number of the parameters, depending on the data that is required. Section I deals with single parameter search. Section II explains how to search with two or more parameters.

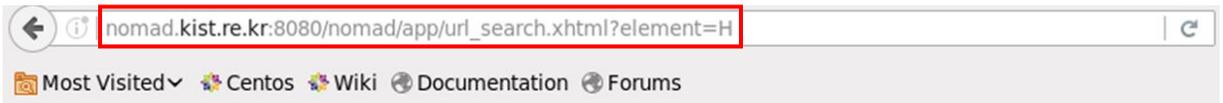
I. Single Parameter Search

A. Search with a single element, for example 'H'

- i. Type the application URL with a question mark at the end in a browser



- ii. Type the 'element=H' after the URL



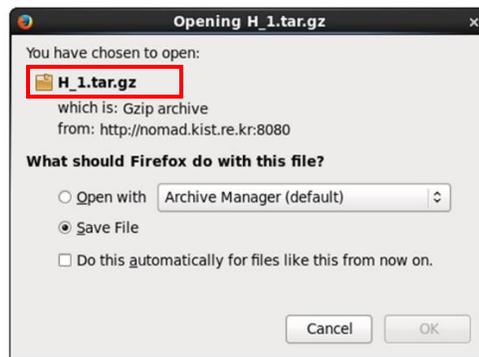
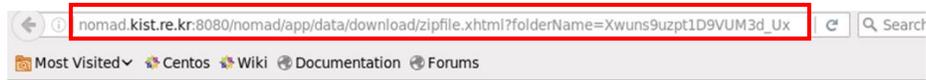
- iii. Press the 'Enter' on the keyboard and wait for the search to complete. The list of retrieved files will be listed in the browser window.



- iv. The downloadable link has three parts

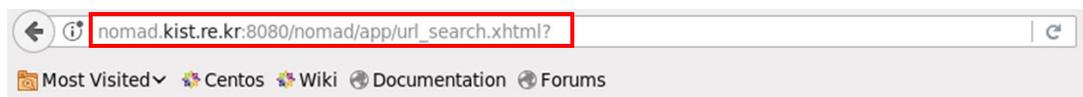
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- [http://nomad.kist.re.kr:8080/nomad/app/data/download/zipfile.xhtml?](http://nomad.kist.re.kr:8080/nomad/app/data/download/zipfile.xhtml?folderName=Xwuns9uzpt1D9VUM3d_UxuE0XofRnmXqOTeWDAFI&file)
– the downloadable links are temporarily stored on this page
 - folderName=Xwuns9uzpt1D9VUM3d_UxuE0XofRnmXqOTeWDAFI&file
- the folder which contains the files
 - Name=H_1 – The name for the Download. A sequential list of downloadable files starting with the search element
- v. Copy any of the file links into the address bar of a browser and press ‘Enter’ to download the files

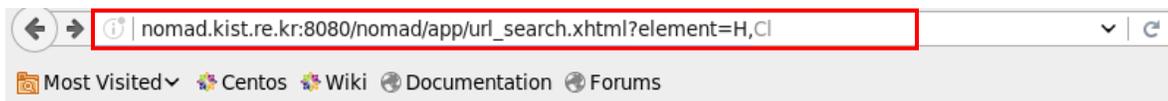


B. Search with multiple (two or more) elements, for example Hydrogen(H) and Chlorine(Cl)

- i. Type the application URL with a question mark at the end in a browser

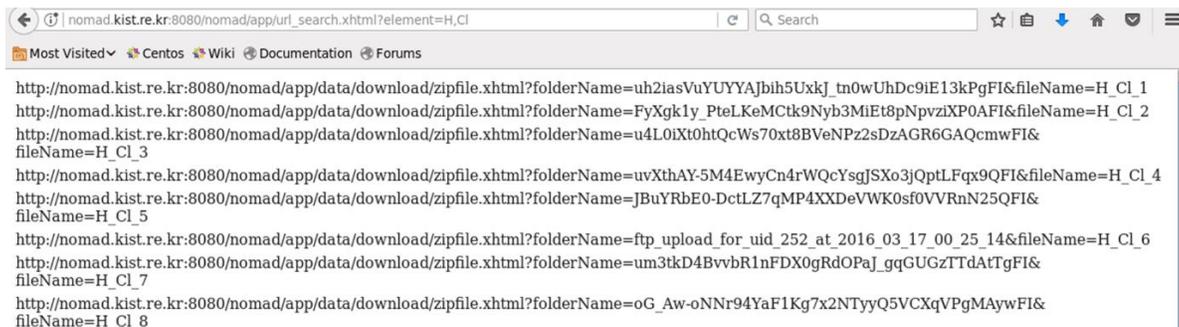


- ii. Type ‘element=H,Cl’ after the URL. The elements should be separated by a comma only without any spaces

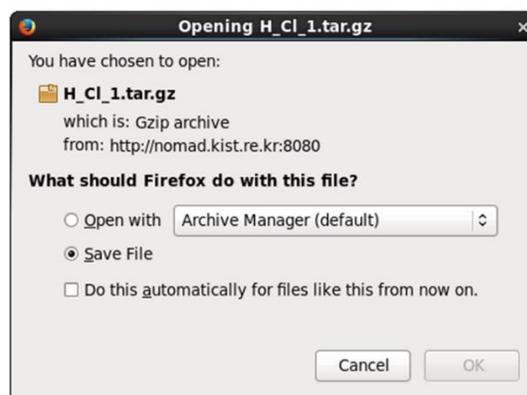
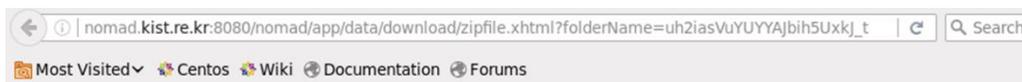


iii. Press the 'Enter' on the keyboard and wait for the search to complete.

The list of retrieved files will be listed in the browser window.

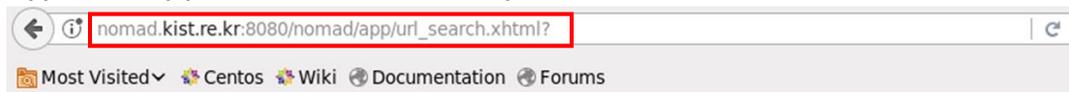


iv. Copy any of the file links into the address bar of a browser and press 'Enter' to download the files

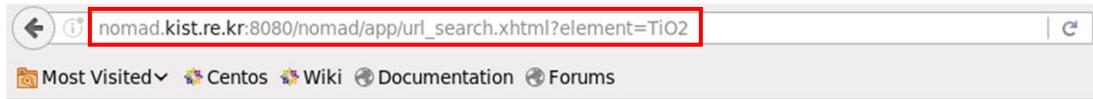


C. Search with a chemical formula, for example 'TiO2'

i. Type the application URL with a question mark at the end in a browser



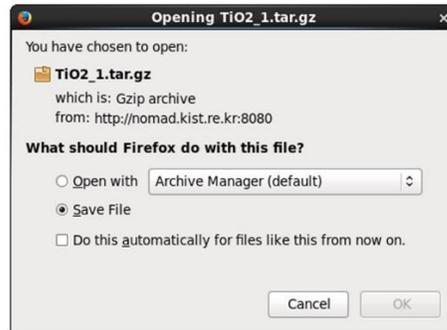
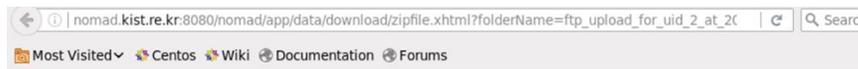
ii. Type 'element=TiO2' after the URL



- iii. Press the 'Enter' on the keyboard and wait for the search to complete. The list of retrieved files will be listed in the browser window

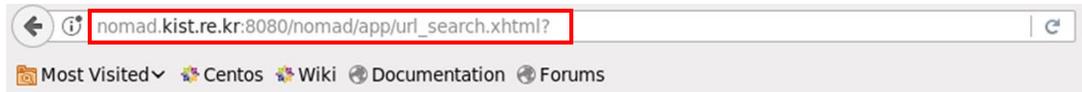


- iv. Copy any of the file links into the address bar of a browser and press 'Enter' to download the files

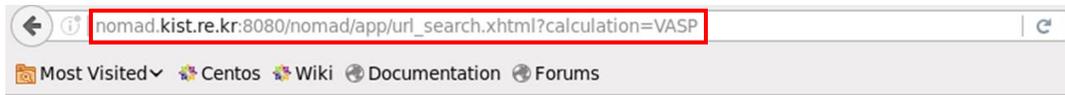


D. Search with a calculation method, for example 'VASP'

- i. Type the application URL with a question mark at the end in a browser



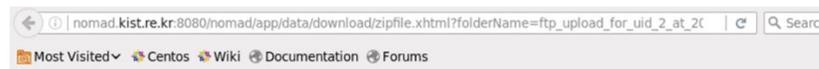
- ii. Type 'calculation=VASP' after the URL



- iii. Press the 'Enter' on the keyboard and wait for the search to complete.
The list of retrieved files will be listed in the browser window

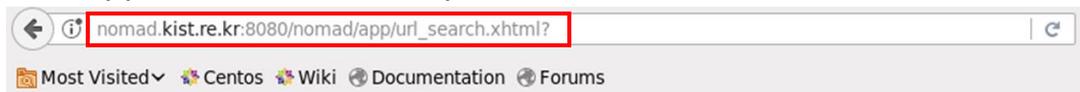


- iv. Copy any of the file links into the address bar of a browser and press 'Enter' to download the files

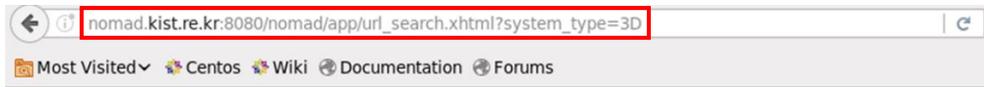


E. Search with a particular system type, for example '3D'

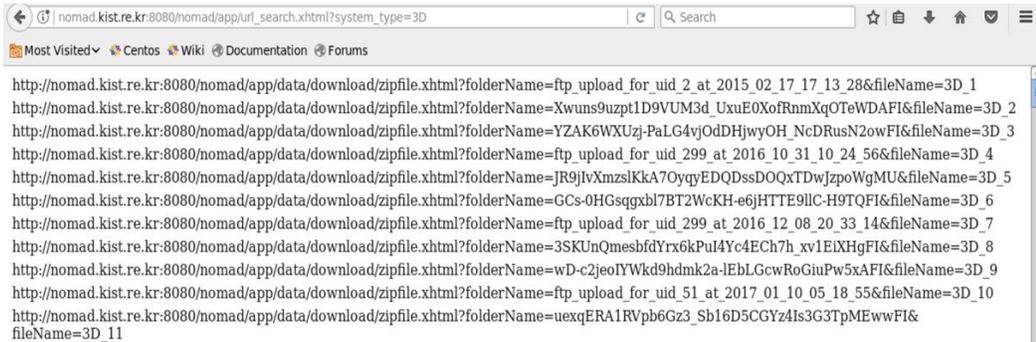
- i. Type the application URL with a question mark at the end in a browser



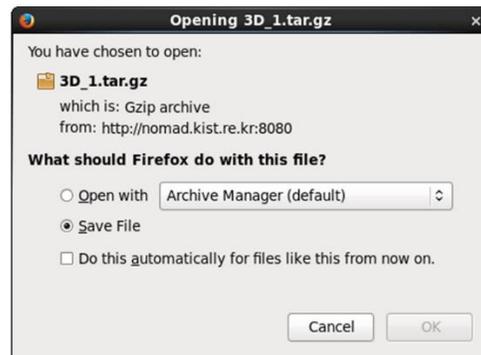
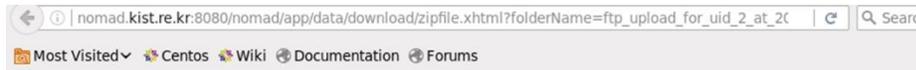
- ii. Type 'system_type=3D' after the URL



iii. Press the 'Enter' on the keyboard and wait for the search to complete. The list of retrieved files will be listed in the browser window

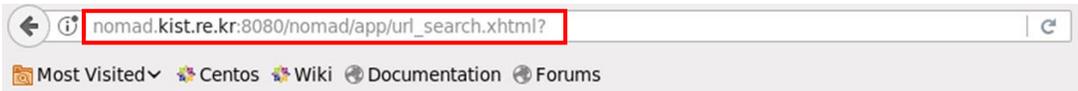


iv. Copy any of the file links into the address bar of a browser and press 'Enter' to download the files

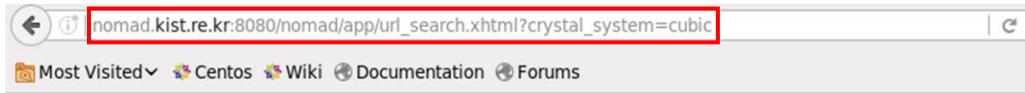


F. Search with a particular crystal system type, for example 'cubic'

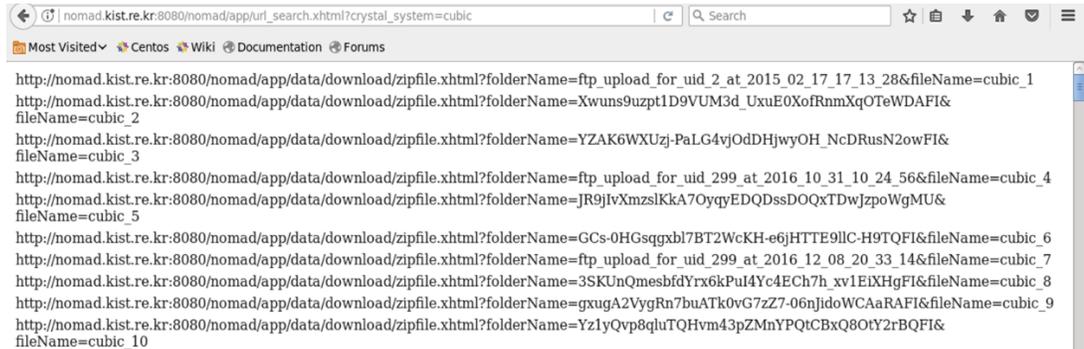
i. Type the application URL with a question mark at the end in a browser



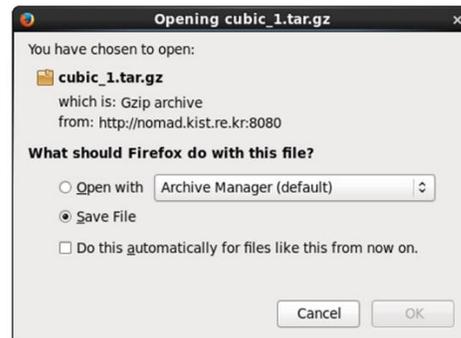
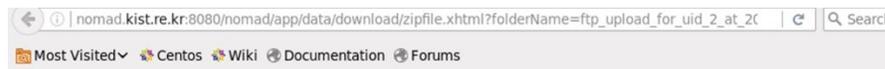
ii. Type 'crystal_system=cubic' after the URL



- iii. Press the 'Enter' on the keyboard and wait for the search to complete. The list of retrieved files will be listed in the browser window

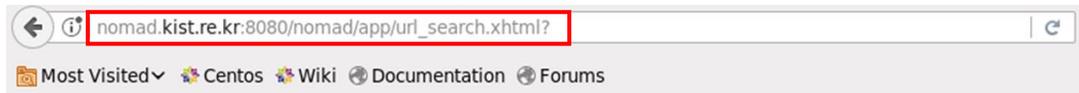


- iv. Copy any of the file links into the address bar of a browser and press 'Enter' to download the files

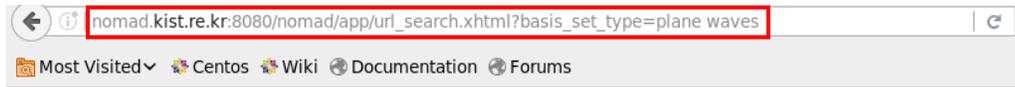


G. Search with a particular basis set type, for example 'plane waves'

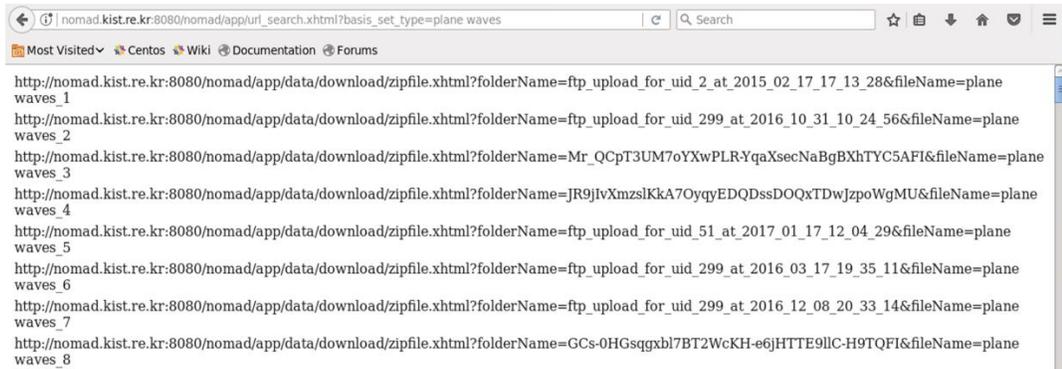
- i. Type the application URL with a question mark at the end in a browser



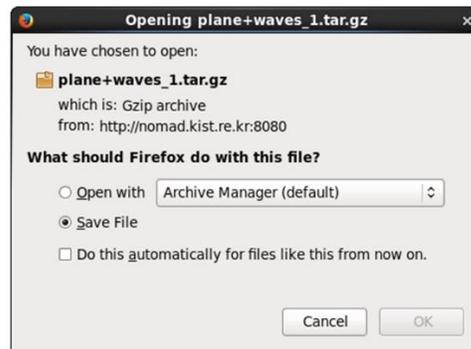
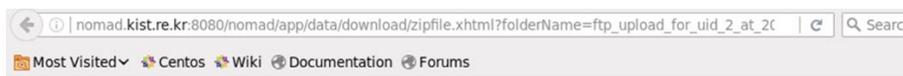
- ii. Type 'basis_set_type=plane waves' after the URL



- iii. Press the 'Enter' on the keyboard and wait for the search to complete. The list of retrieved files will be listed in the browser window

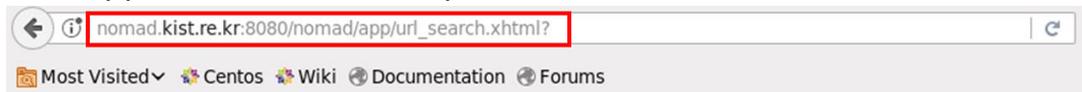


- iv. Copy any of the file links into the address bar of a browser and press 'Enter' to download the files

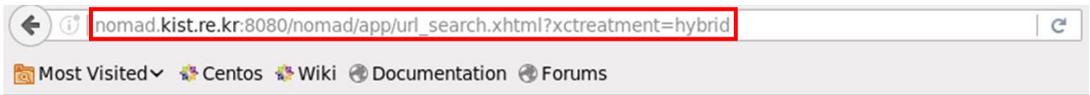


H. Search with a particular xc treatment type, for example 'hybrid'

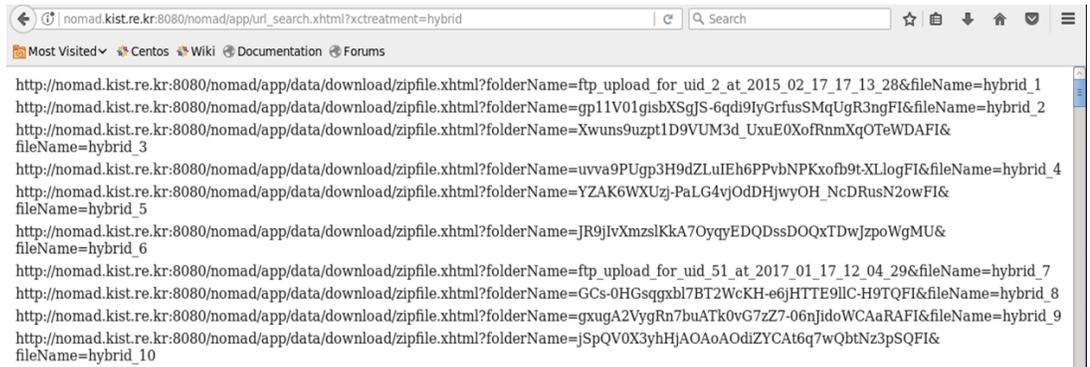
- i. Type the application URL with a question mark at the end in a browser



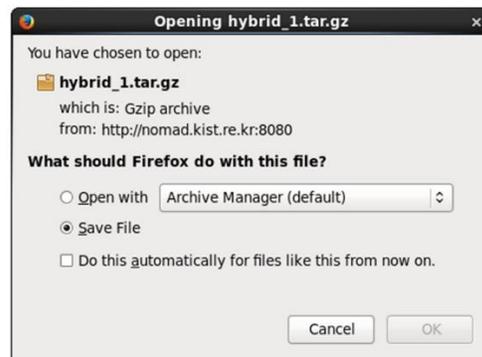
- ii. Type 'xctreatment=hybrid' after the URL



iii. Press the 'Enter' on the keyboard and wait for the search to complete. The list of retrieved files will be listed in the browser window

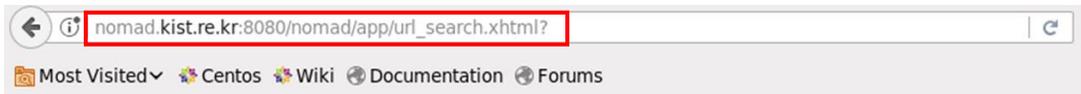


iv. Copy any of the file links into the address bar of a browser and press 'Enter' to download the files

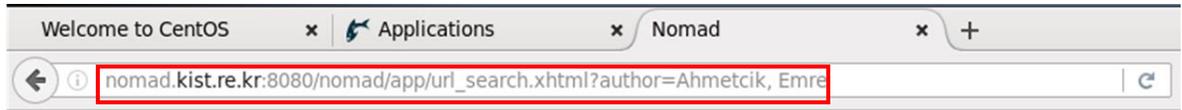


I. Search with a particular author, for example 'Emre Ahmetcik'

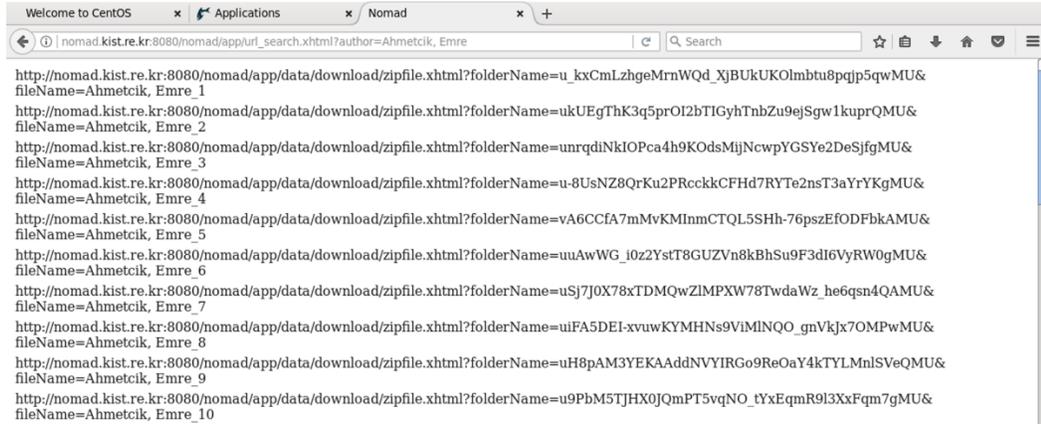
i. Type the application URL with a question mark at the end in a browser



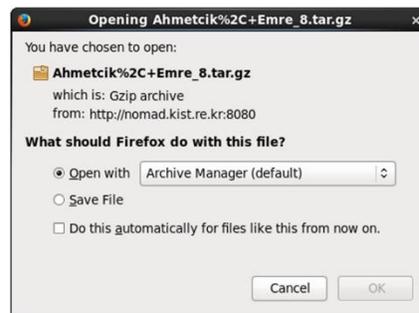
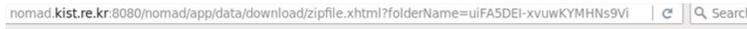
ii. Type 'author= Ahmetcik, Emre' after the URL



- iii. Press the 'Enter' on the keyboard and wait for the search to complete. The list of retrieved files will be listed in the browser window



- iv. Copy any of the file links into the address bar of a browser and press 'Enter' to download the files

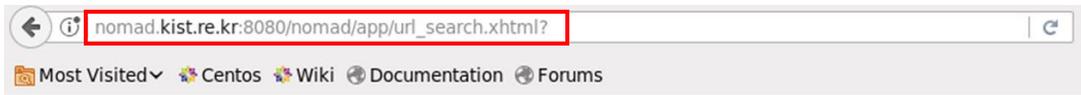


II. Search with two or more parameters

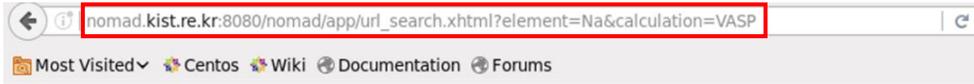
Users can search with any combination of the search parameters

- A. Search with two parameters: element and calculation method, for example element 'Na' and calculation method 'VASP'

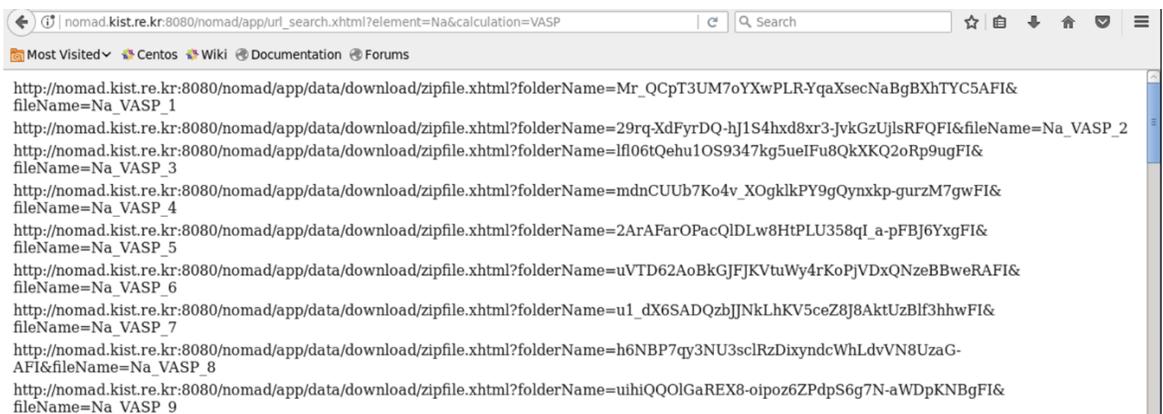
- i. Type the application URL with a question mark at the end in a browser



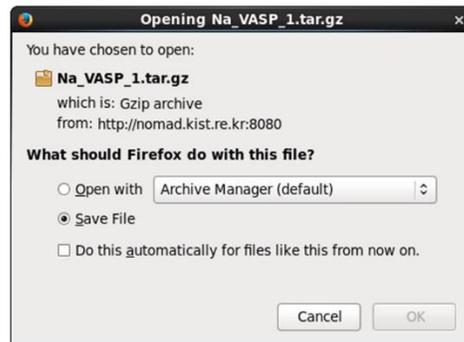
- ii. Type 'element=Na&calculation=VASP' after the URL. Note that the search parameters are joined with the '&' and there should be no space in between



- iii. Press the 'Enter' on the keyboard and wait for the search to complete. The list of retrieved files will be listed in the browser window

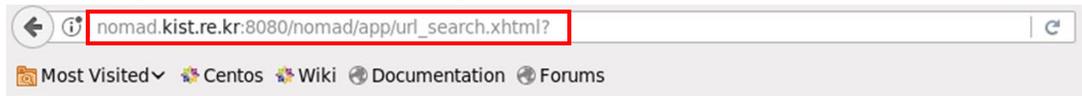


- iv. Copy any of the file links into the address bar of a browser and press 'Enter' to download the files

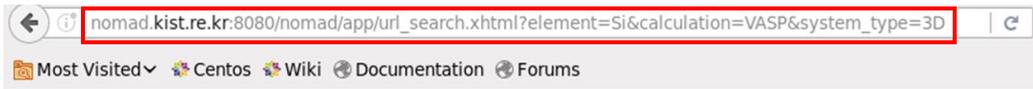


- B. Search with three parameters: element, calculation method and system type. For example, element 'Si', calculation 'VASP' and system_type '3D'

i. Type the application URL with a question mark at the end in a browser

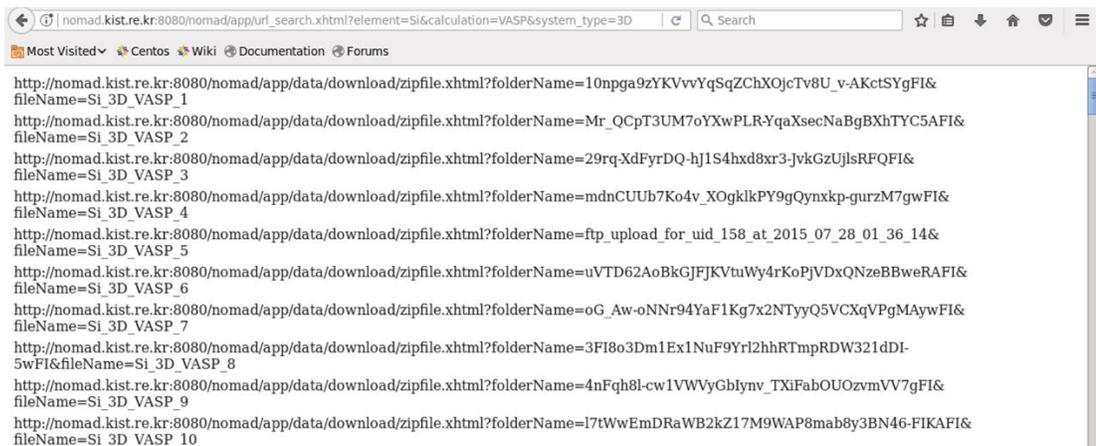


ii. Type 'element=Si&calculation=VASP&system_type=3D' after the URL



iii. Press the 'Enter' on the keyboard and wait for the search to complete.

The list of retrieved files will be listed in the browser window

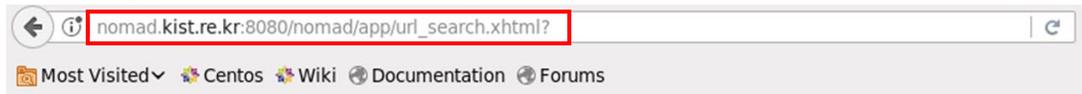


iv. Copy any of the file links into the address bar of a browser and press 'Enter' to download the files

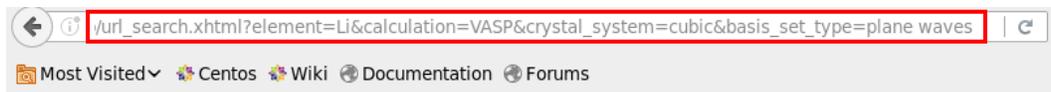


C. Search with four parameters: element, calculation method, crystal system type and basis set type. For example, element 'Li', calculation 'VASP' and crystal_system 'cubic' and basis_set_type 'plane waves'

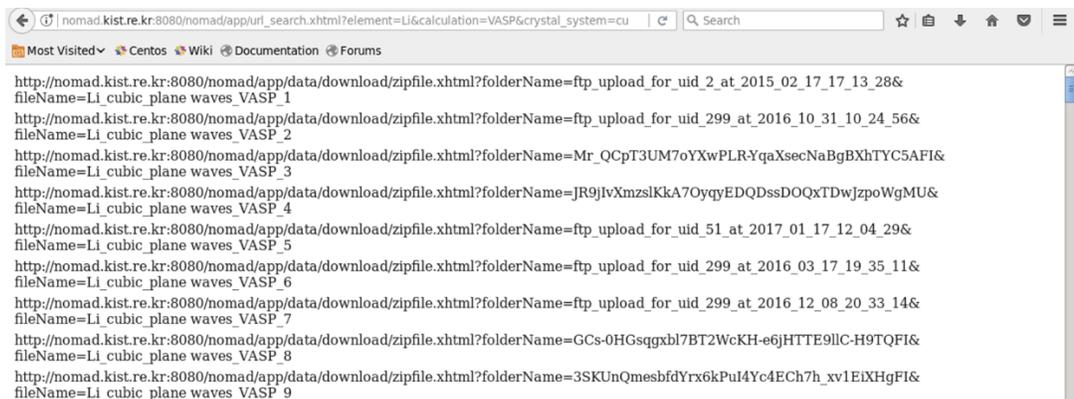
- i. Type the application URL with a question mark at the end in a browser



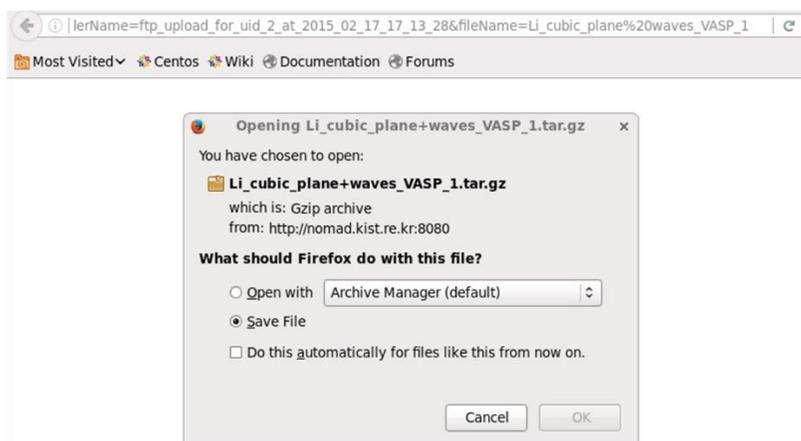
- ii. Type
'**element=Li&calculation=VASP&crystal_system=cubic&basis_set_type=plane waves**' after the URL



- iii. Press the 'Enter' on the keyboard and wait for the search to complete.
The list of retrieved files will be listed in the browser window

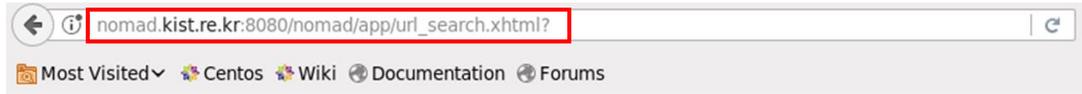


- iv. Copy any of the file links into the address bar of a browser and press
'Enter' to download the files



D. Search with five parameters: crystal system, system type, calculation, basis set type and xc treatment. For example, calculation 'VASP' and crystal_system 'cubic', basis_set_type 'plane waves', system_type '3D' and xctreatment 'GGA'

i. Type the application URL with a question mark at the end in a browser

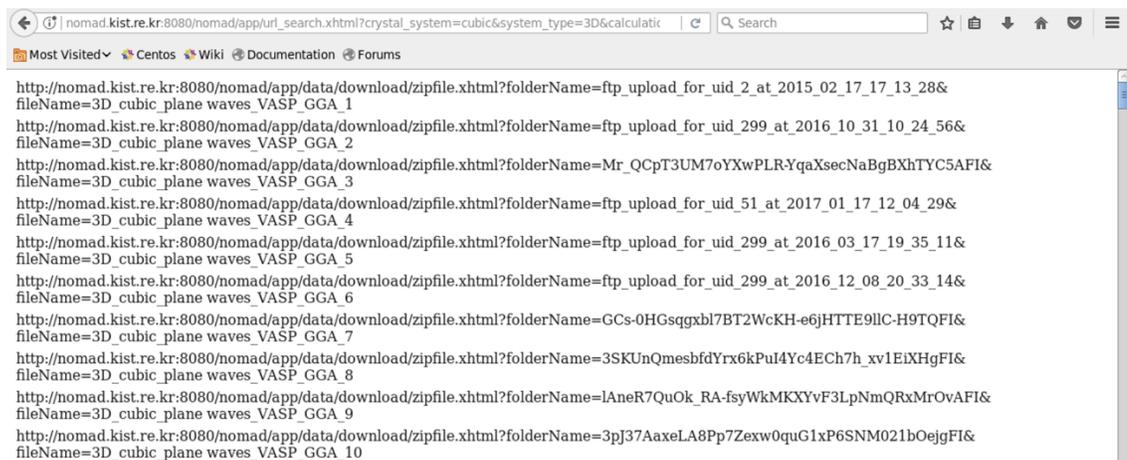


ii. Type

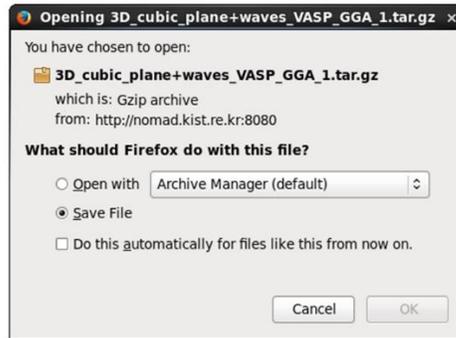
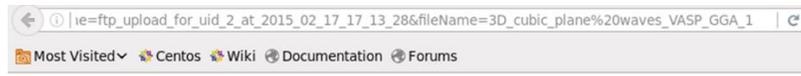
'crystal_system=cubic&system_type=3D&calculation=VASP&basis_set_type=plane waves&xctreatment=GGA' after the URL



iii. Press the 'Enter' on the keyboard and wait for the search to complete. The list of retrieved files will be listed in the browser window

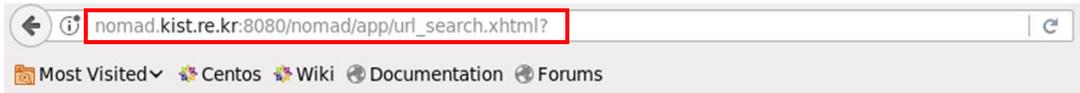


iv. Copy any of the file links into the address bar of a browser and press 'Enter' to download the files



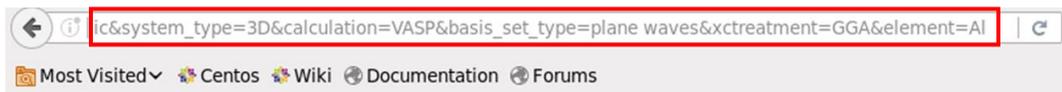
E. Search with six parameters: element, crystal system, system type, calculation, basis set type and xc treatment. For example, element=Al, calculation 'VASP' and crystal_system 'cubic', basis_set_type 'plane waves', system_type '3D' and xctreatment 'GGA'

i. Type the application URL with a question mark at the end in a browser

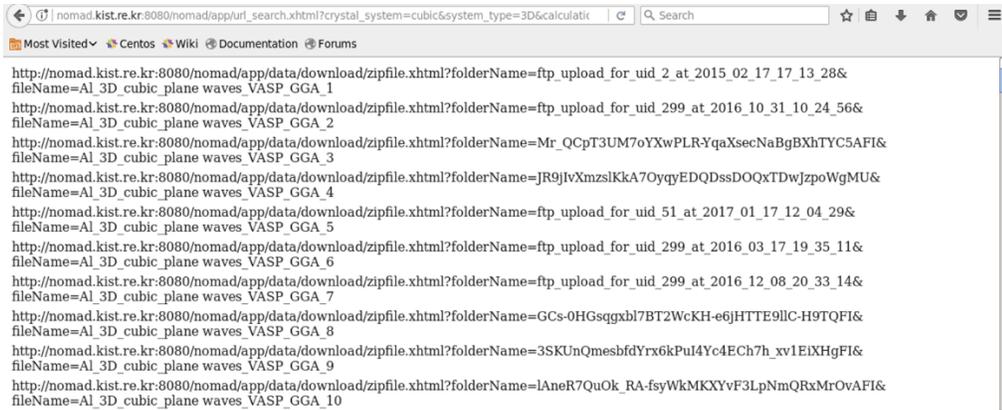


ii. Type

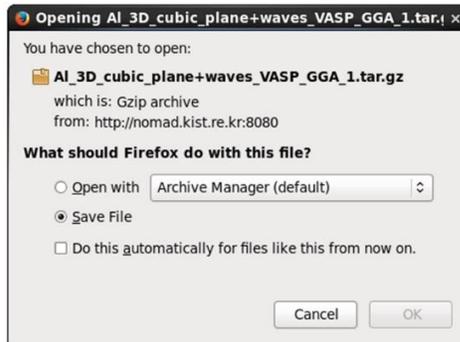
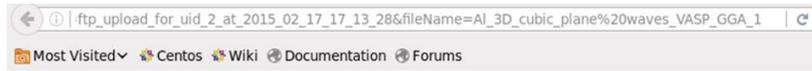
'crystal_system=cubic&system_type=3D&calculation=VASP&basis_set_type=plane waves&xctreatment=GGA&element=Al' after the URL



iii. Press the 'Enter' on the keyboard and wait for the search to complete. The list of retrieved files will be listed in the browser window



iv. Copy any of the file links into the address bar of a browser and press 'Enter' to download the files



References

- i. The NOMAD Laboratory. A European Centre of Excellence. Website: <https://www.nomad-coe.eu/>
- ii. The NOMAD Repository. Website: <https://repository.nomad-coe.eu/>