

This example was created by Omar using this link for vaspkit : <https://vaspkit.com/tutorials.html>:

The use of vaspkit is for postprocessing data or creating input cards

First to create a MD , relax incar we load vaspkit by typing on your terminal vaspkit.

Example:

Type vaspkit

```
[omf071@plato1gn001 NEBExample]$ vaspkit
[mii] loading StdEnv/2023 vaspkit/1.5.1 ...

  \\\\//
 /  _  \      Hey, you must know what you are doing.
(| (o) (o) |)  Otherwise you might get wrong results.
o-----.000o-- () --o000.-----o
|          VASPKIT Standard Edition 1.5.1 (27 Jan. 2024)          |
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|          Main Contributors: Gang TANG, Nan XU & Jin-Cheng LIU   |
|          Online Tutorials Available on Website: https://vaspkit.com |
o-----.0000-----o
  ( )      Oooo.          VASPKIT Made Simple
  \ (      ( )
  \_)     ) /
         ( /

===== Structural Utilities =====
01) VASP Input-Files Generator      02) Mechanical Properties
03) K-Path for Band-Structure      04) Structure Editor
05) Catalysis-ElectroChem Kit     06) Symmetry Analysis
07) Materials Databases           08) Advanced Structure Models
===== Electronic Utilities =====
11) Density-of-States             21) Band-Structure
23) 3D Band-Structure            25) Hybrid-DFT Band-Structure
26) Fermi-Surface                28) Band-Structure Unfolding
31) Charge-Density Analysis       42) Potential Analysis
44) Piezoelectric Properties      51) Wave-Function Analysis
62) Magnetic Analysis            65) Spin-Texture
68) Transport Properties

===== Misc Utilities =====
71) Optical Properties            72) Molecular-Dynamics Kit
74) User Interface               78) VASP2other Interface
84) ABACUS Interface             91) Semiconductor Kit
92) 2D-Material Kit             95) Phonon Analysis
0) Quit
----->>
```

After loading vaspkit will display various options with number in front of each properties. To choose a property write the number in front of the property like: 01) VASP Input-Files Generator

## Example

We Type 1 in the terminal and you will get these options:

```
1
===== VASP Input Files Options =====
101) Customize INCAR File
102) Generate KPOINTS File for SCF Calculation
103) Generate POTCAR File with Default Setting
104) Generate POTCAR File with User Specified Potential
105) Generate POSCAR File from cif (no fractional occupations)
106) Generate POSCAR File from Material Studio xsd (retain fixes)
107) Reformat POSCAR File in Specified Order of Elements
108) Successive Procedure to Generate VASP Files and Check
109) Submit Job Queue

0)  Quit
9)  Back
----->>
```

If you want to generate INCAR type 101 on the terminal you will get this:

```
----->>
101) Customize INCAR File
+----- Tip -----+
|           WARNING: You MUST know what you are doing!           |
|Some Parameters in INCAR file need to be set/adjusted manually. |
+-----+
===== INCAR Options =====
ST) Static-Calculation          SR) Standard Relaxation
MG) Magnetic Properties        SO) Spin-Orbit Coupling
D3) DFT-D3 no-damping Correction H6) HSE06 Calculation
PU) DFT+U Calculation          MD) Molecular Dynamics
GW) GW0 Calculation            BS) BSE Calculation
DC) Elastic Constant           EL) ELF Calculation
BD) Bader Charge Analysis      OP) Optical Properties
EC) Static Dielectric Constant PC) Decomposed Charge Density
PH) Phonon-Calculation         PY) Phonon with Phonopy
NE) Nudged Elastic Band (NEB)  DM) The Dimer Method
FQ) Frequency Calculation      LR) Lattice Relaxation
MT) Meta-GGA Calculation       PZ) Piezoelectric Calculation

0)  Quit
9)  Back
----->>
Input Key-Parameters (STH6D3 means HSE06-D3 Static-Calculation)
```

From this stage you type the two let for the calculation you want to perform;  
Type ST on the terminal to get the final input.

```
Input key=Parameters (SIRODS means HSE06-D3 Static-Calculation)
ST
-->> (01) Written INCAR file!
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|          * ACKNOWLEDGMENTS *          |
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| Ya-Chao LIU, Jiang-Shan ZHAO, Qi-Jing ZHENG, Yue QIU and You! |
| Advisors: Wen-Tong GENG, Yoshiyuki KAWAZOE |
| :) Any Suggestions for Improvement are Welcome and Appreciated (: |
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|          * CITATIONS *          |
| When using VASPKIT in your research PLEASE cite the paper: |
| [1] V. WANG, N. XU, J.-C. LIU, G. TANG, W.-T. GENG, VASPKIT: A |
| User-Friendly Interface Facilitating High-Throughput Computing |
| and Analysis Using VASP Code, Computer Physics Communications |
| 267, 108033, (2021), DOI: 10.1016/j.cpc.2021.108033 |
|-----o
[omf071@plato1gn001 NEBExample]$ █
```