

Parameter Input File

input.txt: this is the file which feeds simulation parameters from the user into *CrystalGrower* at runtime. Values in this file determine which structure will be grown and under what conditions / additional growth factors (e.g. screw dislocations).

input.txt contains all the main parameters to be loaded into *CrystalGrower*. This is the first file which is required for every *CrystalGrower* run. When using the graphical user interface (GUI) version of *CrystalGrower*, this file is generated automatically and populated by the user responses to questions. This section presents an example (along with a labelled example) for an input.txt file.

(Note that the filename for this file must always be input.txt and must be located in the same directory as the CrystalGrower executable for the command line version of CrystalGrower).

Example

- 1) ./Simulations/Test/
- 2) 11_MOF-5
- 3) no
- 4) ./Simulations/Test/10_MOF-5_checkpoint.txt
- 5) yes
- 6) ./Structure_Files/Molecular/MOF-5.txt
- 7) normal
- 8) no
- 9) 1
- 10) 1
- 11) yes
- 12) yes
- 13) 10000
- 14) 180.00
- 15) 1000000
- 16) 2
- 17) no
- 18) 0.000
- 19) 1
- 20) 1

- 21) 1000000
- 22) 1000
- 23) 1
- 24) 1000000
- 25) no
- 26) ./Simulations/Test/10_MOF-5_colouring.txt

General Example

- 1) Directory to store data - Path to the directory where the simulation output will be saved.
- 2) File root to store data - The root filename that will be assigned to all simulation output files.
- 3) Do you want to load a checkpoint to start your simulation? (yes/no) - enables or disables the use of a previous simulation as a starting point for the next simulation (i.e. reading in a seed crystal).
- 4) File path for checkpoint load - pathway to the checkpoint file to read in as a seed (N/A if the answer to the previous question is no, however data is still required on this line when the file is read into *CrystalGrower*).
- 5) Do you want to save a checkpoint at the end of your simulation? (yes/no) - creates a checkpoint file that can be read into other simulations as a seed with the filename `Root_checkpoint.txt`, saved in directory with simulation output.
- 6) File path to structure file: e.g. `../LTA.txt` (Must be a text file) - Pathway to read in the structure file that defines which crystal structure is to be grown.
- 7) Operation mode of the program? (normal / growth_modifier / ordered / screw_stress) - “normal” is the standard *CrystalGrower* operation mode, “growth_modifier” enables the addition of poisons or growth modifiers, “ordered” allows energy penalties to be assigned to tile vertices with different atom types e.g. Si or Al, “screw_stress” allows the users to model the slower growth at screw dislocation cores which caused by crystal strain by poisoning the growth near the screw core. Users will be asked follow-up questions for the “growth_modifier” operation mode to specify sites to poison, the frequency to poison and the residence time of the poison / growth modifier. Follow-up questions will be asked for the “ordered” operation mode to specify the tile vertex atom types to affect, along with the energy penalty for said vertices. Follow-up questions for “screw_stress” will be similar to the “growth_modifier” option

(frequency and residence time of a poison / modifier) along with specifying a radius from the screw core where poisons / modifiers can attached.

- 8) Do you want to add a screw dislocation? (yes / no) - activates a single screw dislocation, users will be asked follow-up questions to specify screw core direction and Burgers vector.
- 9) How many checking sweeps, 1 is normal, 2 to clear internal defects. 1 or 2? - 1 sweep will be sufficient for all systems unless internal defects are under study. 2 will enable a second neighbour sweep to eliminate all redundant defects.
- 10) Method for determining multipliers for combinations. 1 or 2? - Select different methods for calculating the number of combinations of coordinations for site types. 1 should be used unless the system is too complex, where 2 should be invoked.
- 11) Is this a tile or net crystal? (tile / net) - "tile" constructs the crystal using natural tiles, this option should be used for cage structures e.g. zeolites or other nanoporous materials (excluding MOFs). "net" treats the crystal structure as a molecular / ionic crystal, where the units of growth are individual ions / molecules.
- 12) Do you want to calculate the required memory for running your calculation? (yes / no) - "yes" will automatically calculate the memory required to grow the crystal under the desired conditions, by calculating growth rates in the *a*, *b* and *c* directions. "no" will allow the user to manually specify the size of the simulation space in unit cells in the *a*, *b* and *c* directions through follow up questions (dimensions must be odd-numbered integers).
- 13) What is the maximum memory in MBytes that you wish to use? (Recommended default 10000 Mbytes) - Sets the limit for memory allocation in megabytes, if *CrystalGrower* is calculated to require more than this amount it will issue a warning and stop the simulation.
- 14) Temperature in Celsius? - System temperature in Celsius for the simulation.
- 15) Number of iterations? (Must be an integer)? - The length of the simulation in iterations. One iteration is a single growth or dissolution event, this parameter is correlated to the length of the simulation.
- 16) Delta mu mode? - the reaction profile that the solution follows during the simulation. Figures for each mode (1-7) are shown in another part of this manual.
- 17) Do you want an excess supersaturation of any component (always yes for a MOF)? yes/no - "yes" will enable setting an excess supersaturation / delta

μ for each species in the system separately. This value is an offset, and will add to the base supersaturation defined by the delta μ mode and starting / new delta μ values input by the user. Setting -1 as an excess value will set a constant +10 kcal / mol excess that follows the delta μ mode and is intended to represent the excess for a solvent species included in the crystal structure e.g. in a MOF. "no" will restrict all species to only the base supersaturation value for the system.

- 18) Starting delta μ [kcal/mol]? - The starting value for the base delta μ in kcal / mol for the system.
- 19) MOVIE: The number of frames? (must be an integer) - Number of simulation frames that are output for visualisation. Frames are equally spaced between the answers to the following two questions.
- 20) MOVIE: Iteration at movie capture start? (default is 1) (must be an integer) - The number of iterations where you want to begin the simulation visualisation capture window.
- 21) MOVIE: Iteration at movie capture end? (default is number of iterations) (must be an integer) - The number of iterations where you want to end the simulation visualisation capture window.
- 22) Delta μ DATA: The number of outputs? (must be an integer) - the number of data points written to the data files output by the simulation. Data points are equally spaced between the answers to the following two questions.
- 23) Delta μ DATA: Iteration at initial output? (default is 1) (must be an integer) - The number of iterations where you want to begin the data point capture window.
- 24) Delta μ DATA: Iteration at final output? (default is number of iterations) (must be an integer) - The number of iterations where you want to end the data point capture window.
- 25) Do you want to visualise crystal terraces? (yes/no) - "yes" will invoke the automatic colouring routine. If the follow-up question is answered with "find" *CrystalGrower* will attempt to identify the facets that are present in the grown crystal and create two output files. One contains all the identified facets, and one contains all possible planes between (4,4,4) and (-4,-4,-4) for this structure. Answering the follow up question with "colour" will instead read in one of these files and use the facets listed in the file to colour the crystal.

26) File path for crystal terrace colouring - The path to the file to read in for colouring the crystal, requires answering "yes" to the previous question then "colour" to the follow up question. When this is not required it is automatically set to "N/A", however data is still required for this line.