How to configure software related with AICON so that it can be run automatically?

1. Configure pymatgen

(1) Change **pymatgen.io.vasp.inputs.Poscar.get_string**, one of its argument **significant_figures: int=11**.

(2) Change **pymatgen.io.vasp.MPRelaxSet.yaml**, one of its argument **POTCAR_FUNCTIONAL: PBE_54**. Also change the default potcar settings in **pymatgen.io.vasp.sets.DictSet**, such as **self.potcar_functional = self._config_dict.get("POTCAR_FUNCTIONAL", "PBE_54")**.

(3) Change the first line in **pymatgen.io.vasp.sets.DictSet.incar**, from *settings = dict(self._config_dict["INCAR"])* to ***settings = dict()***, so that the generated INCAR file is as the user input.

(4) Change **pymatgen.io.vasp.sets.MPStaticSet**, and **pymatgen.io.vasp.sets.MPNonSCFSet**, comment out redundant INCAR settings.

2. Configure Mongodb atlas & pymongo

(1) Register an account on https://www.mongodb.com/atlas/database.

(2) Add the cluster's IP address into the access list of Mongodb atlas.

(3) Create project-cluster-database in atlas, testing the connection between atlas and user cluster using pymongo. Just follow the manual of atlas.

3. Configure atomate and fireworks

(1) Configure necessary files according to https://atomate.org/installation.html#configure-database-connections-and-computing-center-parameters

(2) Change **atomate.vasp.firetasks.run_calc.RunVaspCustodian**, in **handler_groups['default']**, the **UnconvergedErrorHandler()** should be removed. Also, the final return values should be **return FWAction()**, means no vasp run information will be stored in database.

(3) In db.json, use **host_uri** instesd of host.

(4) Change fireworks.core.launchpad.LaunchPad, set **uri_mode=True**. In **if uri_mode** section, set **self.db = self.connection[self.name].**