```
51    # Creating Hamiltonian and initialize it
52    ham = Hamiltonian_Atomistic(1, 3*syst.Number_of_atoms)
53    ham.set_Hamiltonian_type("MM")
54    ham.set_interactions_for_atoms(syst, atlst1, atlst1, uff, 1, 0)  # 0 - verb, 0 - assign_rings
55    ham.show_interactions_statistics()
56
```

This is the template code from the repo directory libra-code\tests\test_md\example_1_SubPc-C60\case1

The parameters are : system object, list of atoms, list of atoms to interact with the ones in the first list, force field object and two boolean values

```
Traceback (most recent call last):
  File "run_aa_md.py", line 112, in <module>
    main()
  File "run_aa_md.py", line 54, in main
    ham.set_interactions_for_atoms(syst, atlst1, atlst1, uff, 1, 0)  # 0 - verb, 0 - assign_rings
Boost.Python.ArgumentError: Python argument types in
    Hamiltonian_Atomistic.set_interactions_for_atoms(Hamiltonian_Atomistic, System, range, range, ForceField, int, int)
did not match C++ signature:
    set_interactions_for_atoms(liblibra::libhamiltonian::libhamiltonian_atomistic::Hamiltonian_Atomistic {lvalue}, liblibra::libchemobjects::libchemsys::System {lvalue}, boost::python::list, boost::python::list,
 liblibra::libforcefield::ForceField {lvalue}, int, int)
```

Here, the function .set_interactions_for_atoms demands an additional parameter named Hamiltonian_Atomistic

```
51  # Creating Hamiltonian and initialize it
52  ham = Hamiltonian_Atomistic(1, 3*syst.Number_of_atoms)
53  ham.set_Hamiltonian_type("MM")
54  ham.set_interactions_for_atoms(MM,syst, atlst1, atlst1, uff, 1, 0)  # 0 - verb, 0 - assign_rings
55  ham.show_interactions_statistics()
56
```

Here, I tried to add MM as the first parameter as the file Hamiltonian_Atomistic.cpp has the code for two types : MM & QM

```
Traceback (most recent call last):
  File "run_aa_md.py", line 112, in <module>
    main()
  File "run_aa_md.py", line 54, in main
    ham.set_interactions_for_atoms(MM,syst, atlst1, atlst1, uff, 1, 0)  # 0 - verb, 0 - assign_rings
NameError: name 'MM' is not defined
(py37) mriganka parasar@LAPTOP-DEJF45RU:/mnt/c/Users/Mriganka Parasar/Libra/libra-code/tests/test_md/example_1_SubPc-C60/case1$
```

This is what I get

This error is common in all the Libra MD code that I have run so far, including the ones where I am using my own force field settings and geometry files.

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