Aim/Hypothesis:

- Study about the NanoParticles and the important features which need to be encountered
- Trying to understand the Converter code and Implementing a converter method for the ISubstance method which is already implemented in the CDK.

Description:

- **Starting of by writing the cdkSubstanceToCMLMolecule method under libio.cml.Convertor:**

```
public CMLMolecule cdkSubstanceToCMLMolecule(ISubstance model) {
      CMLMolecule cmlMolecule = new CMLMolecule();
      cmlMolecule.setConvention("Substance");
        cmlMolecule.setDictRef("cml:Substance");

      return cmlMolecule;
    }
```

- **Ended up with the code below**

```
/*
     * @Author : Sina M. Nick
     * TODO: Check if ontologies are right
     */
    public CMLMolecule cdkSubstanceToCMLMolecule(ISubstance model) {
      CMLMolecule cmlMolecule = new CMLMolecule();
      cmlMolecule.setConvention("Substance");
      cmlMolecule.setDictRef("cml:Substance");

      if(model.getID() != null)
      cmlMolecule.setId(model.getID());
      else
            cmlMolecule.setId("AN ID");

      for (int j = 0; j < model.getAtomContainerCount() ; j++){

            IAtomContainer atoms = model.getAtomContainer(j);
            for (int i = 0; i < atoms.getAtomCount(); i++) {
                  IAtom cdkAtom = atoms.getAtom(i);
                  CMLAtom cmlAtom = cdkAtomToCMLAtom(atoms, cdkAtom);
                  if (atoms.getConnectedSingleElectronsCount(cdkAtom) > 0) {


cmlAtom.setSpinMultiplicity(atoms.getConnectedSingleElectronsCount(cdkAtom) +
1);
                  }
                  cmlMolecule.addAtom(cmlAtom);
            }
            for (int i = 0; i < atoms.getBondCount(); i++) {
                CMLBond cmlBond = cdkBondToCMLBond(atoms.getBond(i));
                cmlMolecule.addBond(cmlBond);
            }

      }
```

```
        return cmlMolecule;
    }
```

- **Not sure if the conversion between a substance to a molecule is the right idea**
- **Since in this case for example if you have two molecules in your substance the bond between them is not encountered.**
- **Maybe the joint ¨moleculeRefs2¨ need to be added to the CDK ¨see http://pubs.acs.org/doi/pdf/10.1021/ci8002123¨**
- **Any ways below you find the test method which was written for this.**

```
@Test
    public void testCdkSubstanceToCMLMolecule() throws IOException {

        IChemObjectBuilder builder = DefaultChemObjectBuilder.getInstance();
        ISubstance substance = builder.newInstance(ISubstance.class);

      //SO3
        IAtomContainer molecule = new AtomContainer();
        Atom S1 = new Atom("S");
        Atom O2 = new Atom("O");
        Atom O3 = new Atom("O");
        Atom O4 = new Atom("O");
        molecule.addAtom(S1);
        molecule.addAtom(O2);
        molecule.addAtom(O3);
        molecule.addAtom(O4);
        Bond b1 = new Bond(S1, O2, IBond.Order.DOUBLE);
        Bond b2 = new Bond(S1, O3, IBond.Order.DOUBLE);
        Bond b3 = new Bond(S1, O4, IBond.Order.DOUBLE);
        molecule.addBond(b1);
        molecule.addBond(b2);
        molecule.addBond(b3);

        substance.addAtomContainer(molecule);

      //XeF4
        IAtomContainer moleculeTwo = new AtomContainer();
        Atom Xe1 = new Atom("Xe");
        Atom F2 = new Atom("F");
        Atom F3 = new Atom("F");
        Atom F4 = new Atom("F");
        Atom F5 = new Atom("F");
        moleculeTwo.addAtom(Xe1);
        moleculeTwo.addAtom(F2);
        moleculeTwo.addAtom(F3);
        moleculeTwo.addAtom(F4);
        moleculeTwo.addAtom(F5);
        Bond b_1 = new Bond(Xe1, F2, IBond.Order.SINGLE);
        Bond b_2 = new Bond(Xe1, F3, IBond.Order.SINGLE);
        Bond b_3 = new Bond(Xe1, F4, IBond.Order.SINGLE);
        Bond b_4 = new Bond(Xe1, F5, IBond.Order.SINGLE);
        moleculeTwo.addBond(b_1);
        moleculeTwo.addBond(b_2);
        moleculeTwo.addBond(b_3);
        moleculeTwo.addBond(b_4);
```

```
        substance.addAtomContainer(moleculeTwo);


      //Molecule  set as Molecule
        IAtomContainer moleculebounder = new AtomContainer();
        Bond MoleculeBound = new Bond(F5,S1);
        moleculebounder.addBond(MoleculeBound);

        substance.addAtomContainer(moleculebounder);

        Convertor convertor = new Convertor(true, null);
        CMLMolecule convertedSubstance =
convertor.cdkSubstanceToCMLMolecule(substance);

        ByteArrayOutputStream out = new ByteArrayOutputStream();

        Serializer serializer = new Serializer(out, "UTF-8");

        serializer.write(new Document(convertedSubstance));

        out.close();

        String expected = "Unkown";
        String actual = new String(out.toByteArray());
        System.out.println(out);
        Assert.assertTrue(actual.contains(expected));

    }
```

- **In order to create the bond between the molecules in this test method a molecule was added a representative of a bond to the substance, however in my opinion this is not the way this should be and the code needs to be extended.**

Results :

The CMLfile created from the elaborated test is shown below :

```
<?xml version="1.0" encoding="UTF-8"?>
<molecule convention="Substance" dictRef="cml:Substance" id="AN ID"
   xmlns="http://www.xml-cml.org/schema">
   <atomArray>
      <atom id="a932951280" elementType="S" formalCharge="0"/>
      <atom id="a1334056213" elementType="O" formalCharge="0"/>
      <atom id="a1753497211" elementType="O" formalCharge="0"/>
      <atom id="a1109537496" elementType="O" formalCharge="0"/>
      <atom id="a542149962" elementType="Xe" formalCharge="0"/>
      <atom id="a141297113" elementType="F" formalCharge="0"/>
      <atom id="a1811148256" elementType="F" formalCharge="0"/>
      <atom id="a1535526014" elementType="F" formalCharge="0"/>
```

```
      <atom id="a1274731299" elementType="F" formalCharge="0"/>
   </atomArray>
   <bondArray>
      <bond id="b1396188371" atomRefs2="a932951280 a1334056213" order="D"/>
      <bond id="b308834266" atomRefs2="a932951280 a1753497211" order="D"/>
      <bond id="b109533863" atomRefs2="a932951280 a1109537496" order="D"/>
      <bond id="b1112079821" atomRefs2="a542149962 a141297113" order="S"/>
      <bond id="b1175371706" atomRefs2="a542149962 a1811148256" order="S"/>
      <bond id="b1917677636" atomRefs2="a542149962 a1535526014" order="S"/>
      <bond id="b973454076" atomRefs2="a542149962 a1274731299" order="S"/>
      <bond id="b1312232486" atomRefs2="a1274731299 a932951280" order="S"/>
   </bondArray>
</molecule>
```