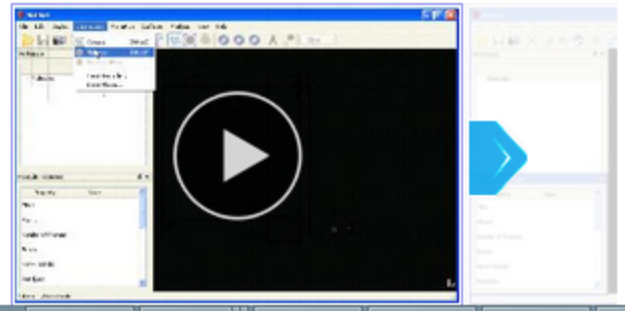
Molekel

Plotting vibrational normal modes

Molekel 5.4 Free

Video tutorial & screenshots



Molekel

- A graphical user interface for plotting in three dimensions
- Molecular orbitals (but we use Pymol)
- Normal modes of vibration

  Procedure uses a program called “calc_freq”.

  Inputs are the files from a vibrational frequency calculation.

  These include .car, .hessian, .grad and .outmol files from the freq calc.

  Use the “vibsave” script to back these up after your frequency calc.

  For example, if you run benzene.job and generate benzene.outmol

  Then you would type $ vibsave benzene

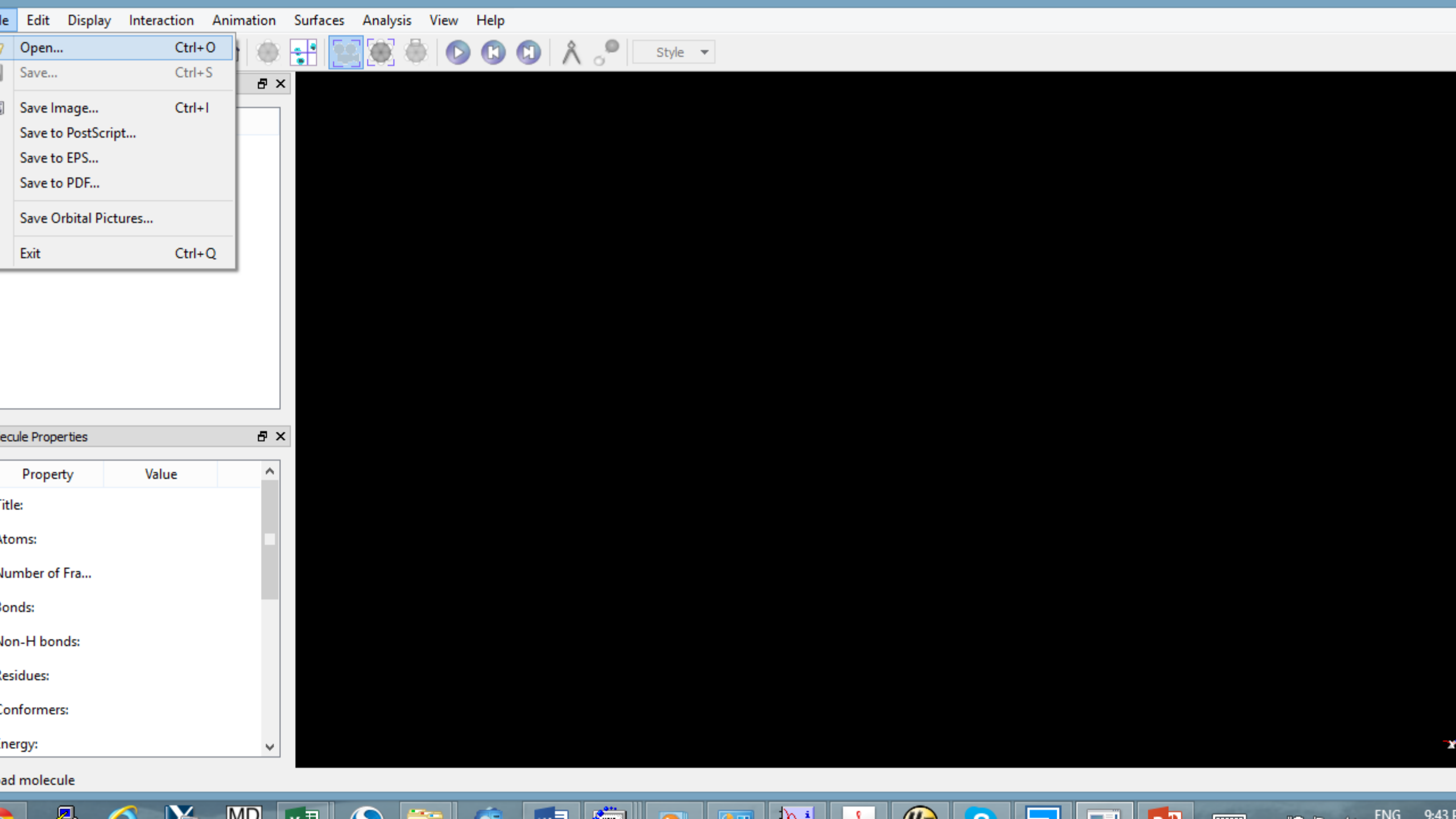
  This will save the appropriate files

- You may copy a script called run_cf_81 from the bin directory.
- You will edit this script so it contains the number of modes you want.
- Then run the script

  $ run_cf_81 benzene

  This will generate xyz files for each mode. Copy these over to your PC

  Run molekel. Select the mode of interest and animate.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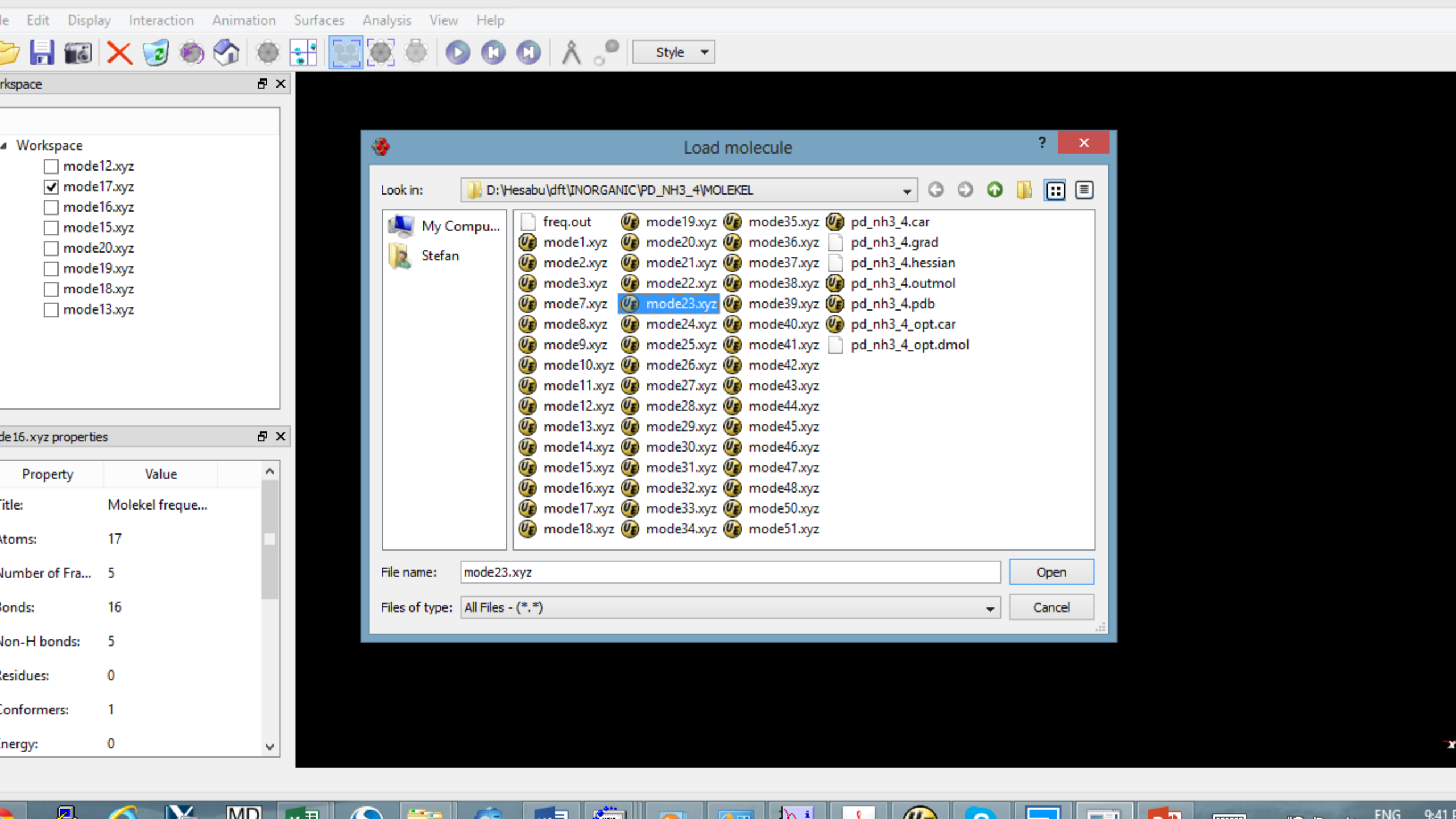
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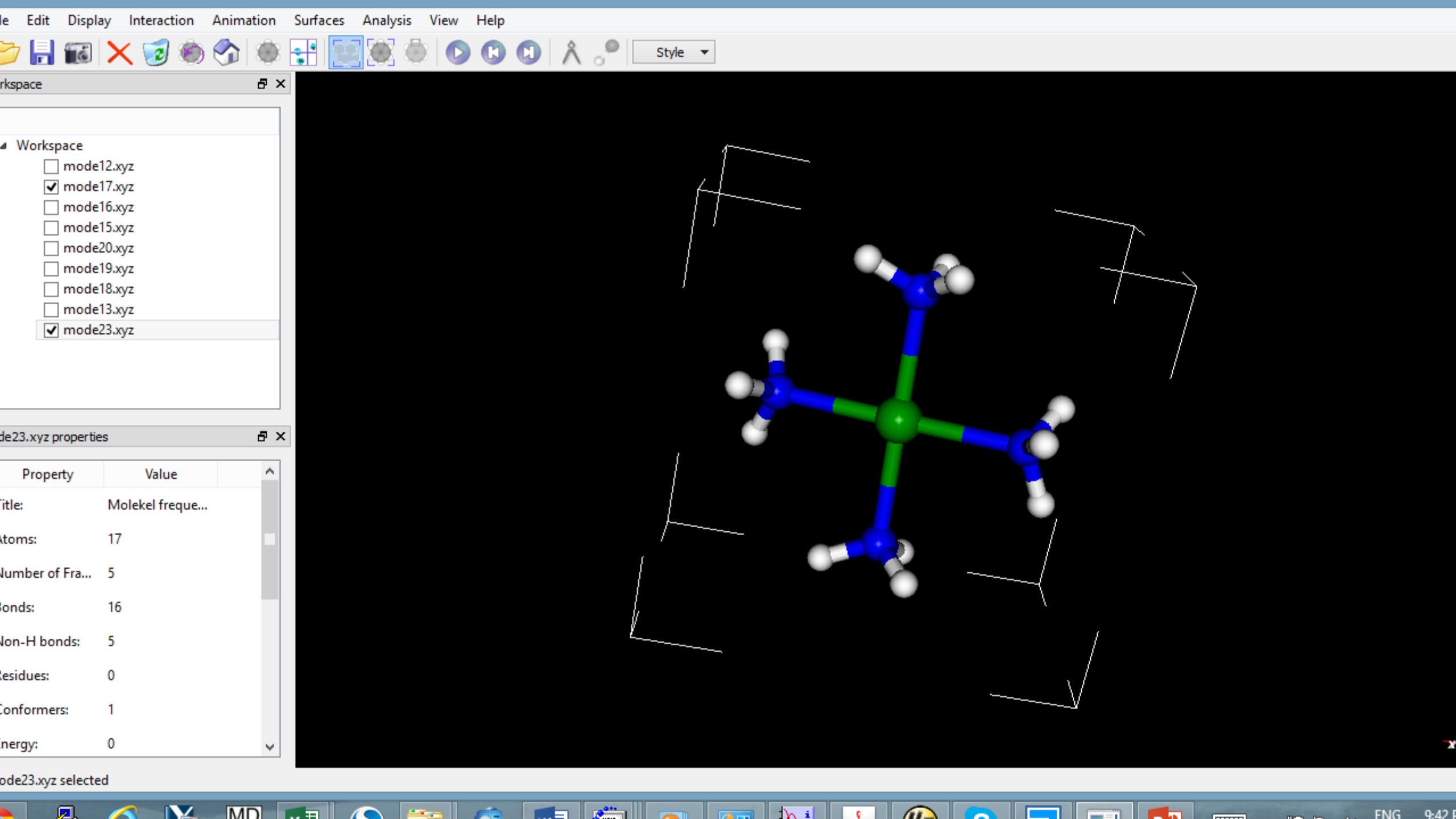
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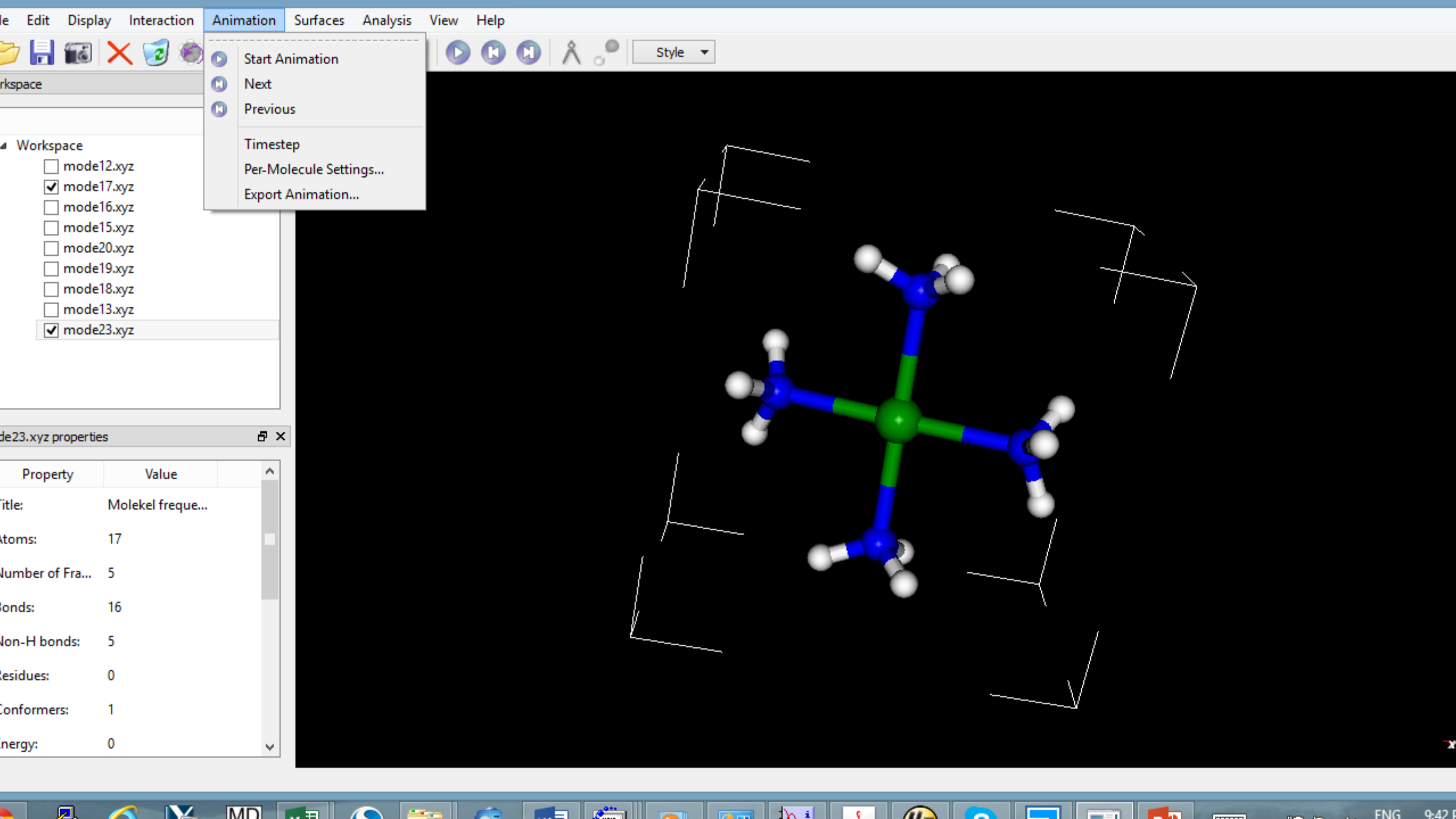
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