

0. CRYSTAL website : <https://www.crystal.unito.it/>

1. CRYSTAL manual :

<https://www.crystal.unito.it/include/manuals/crystal23.pdf>

2. CRYSTAL forum: <https://forum.crystalsolutions.eu/>

3. Tutorial “*A quick tour of CRYSTAL: Wave function calculation input and output*” :

<https://tutorials.crystalsolutions.eu/tutorial.html?td=others&tf=quick>

4. Tutorial “*Introductory Tutorials*” :

[https://tutorials.crystalsolutions.eu/tutorial.html?td=barebone&tf=basic\\_tutorials](https://tutorials.crystalsolutions.eu/tutorial.html?td=barebone&tf=basic_tutorials)

5. Tutorial “*CRYSTAL geometry input*” :

[https://tutorials.crystalsolutions.eu/tutorial.html?td=geometry&tf=geom\\_tut](https://tutorials.crystalsolutions.eu/tutorial.html?td=geometry&tf=geom_tut)

6. Tutorial “*Basis Set Input*” :

[https://tutorials.crystalsolutions.eu/tutorial.html?td=basis\\_set&tf=basis\\_set\\_tut](https://tutorials.crystalsolutions.eu/tutorial.html?td=basis_set&tf=basis_set_tut)

7. Tutorial “*Hamiltonian, computational parameters, SCF & C*” :

[https://tutorials.crystalsolutions.eu/tutorial.html?td=hamil\\_scf&tf=hamil\\_scf\\_tut](https://tutorials.crystalsolutions.eu/tutorial.html?td=hamil_scf&tf=hamil_scf_tut)

8. Tutorial “*Total energy calculation*” :

[https://tutorials.crystalsolutions.eu/tutorial.html?td=totalenergy&tf=total\\_energy\\_tut](https://tutorials.crystalsolutions.eu/tutorial.html?td=totalenergy&tf=total_energy_tut)

9. Moldraw : [https://www.moldraw.unito.it/\\_sgg/f10000.htm](https://www.moldraw.unito.it/_sgg/f10000.htm)
10. Jmol : <https://jmol.sourceforge.net/>
11. OVITO : <https://www.ovito.org/>
12. VESTA : <https://jp-minerals.org/vesta/en/>
13. CRYSPLOT : <https://crysplot.crystalsolutions.eu/index.html>
14. CRYSTAL basis set : [https://www.crystal.unito.it/basis\\_sets.html](https://www.crystal.unito.it/basis_sets.html)
15. Basis set exchange : <https://www.basissetexchange.org/>
16. Stuttgart/Cologne EMS database :  
<https://www.tc.uni-koeln.de/PP/clickpse.en.html>
17. The Materials Project : <https://next-gen.materialsproject.org/>

