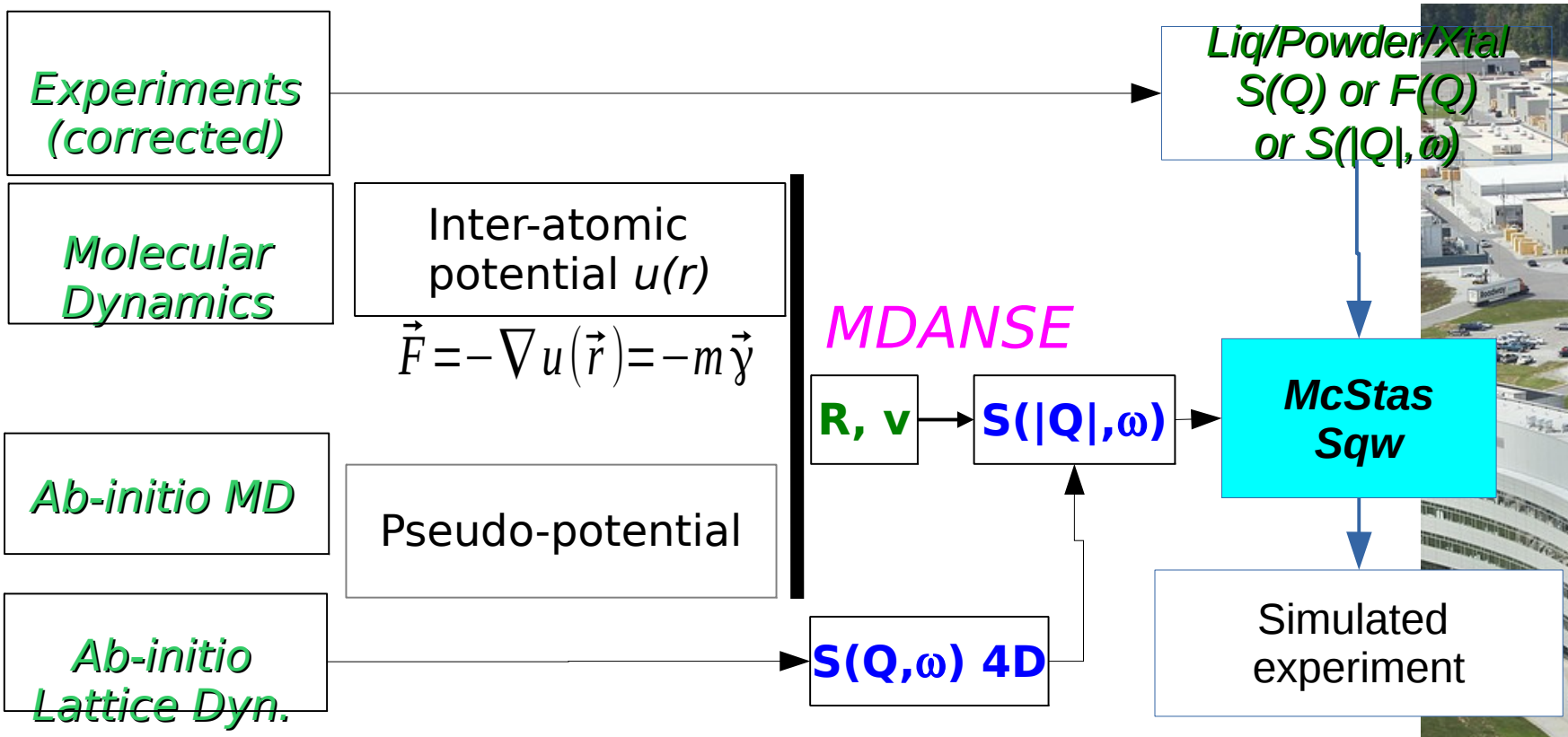
How to get S(q,w) data sets



MD step is done prior to the virtual experiment (NAMD, VASP, GROMACS, ...). Computationally intensive (e.g. use clusters). Then use FFT(r,t)

McStas provides a few sample S(Q,w): Rb, Ge, H2O, D2O, D2, ...

Isotropic_Sqw: Handles **elastic** and **inelastic** for both **coherent** and **incoherent** channels