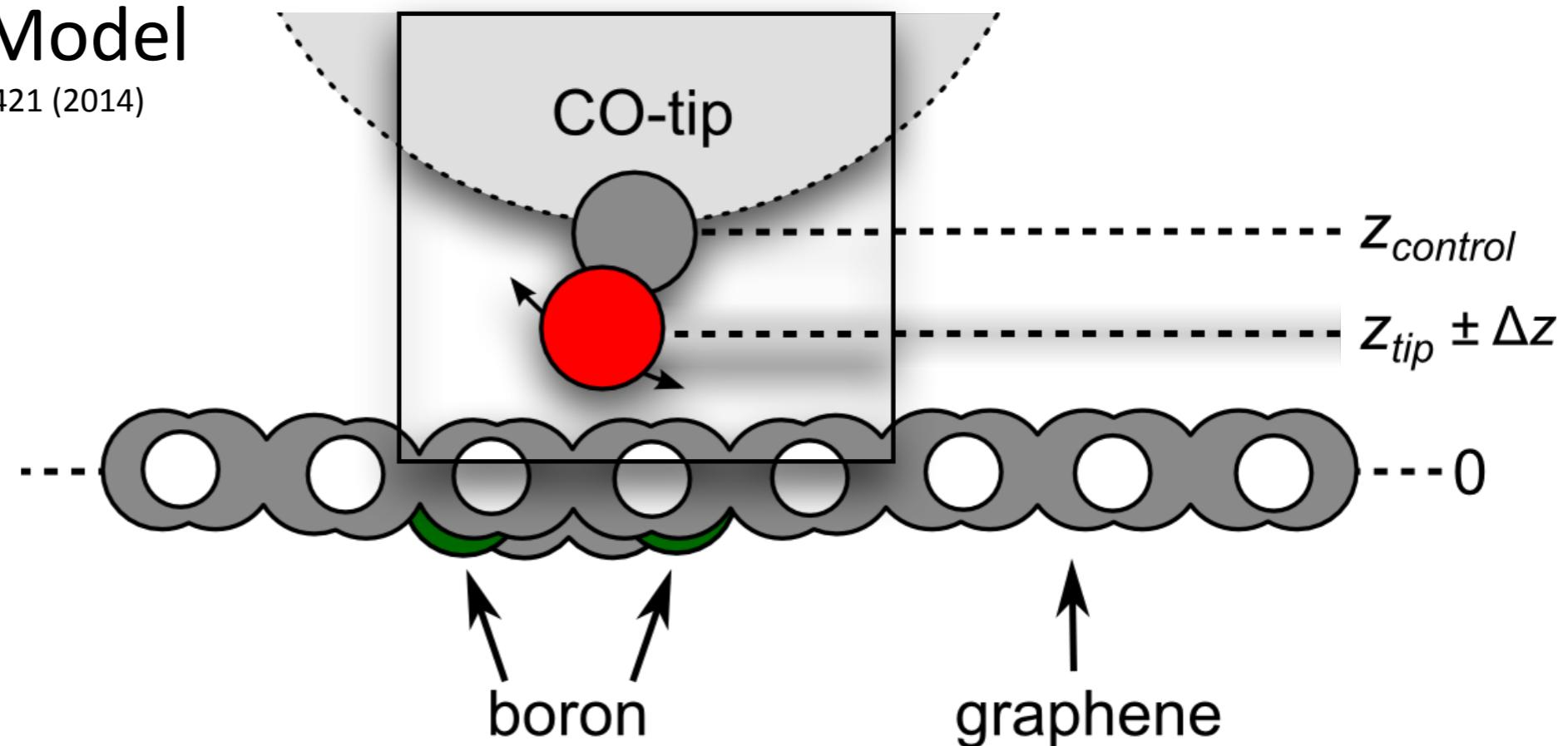


BORON-GRAPHENE-NANORIBBON vAFM

Mechanical AFM Model

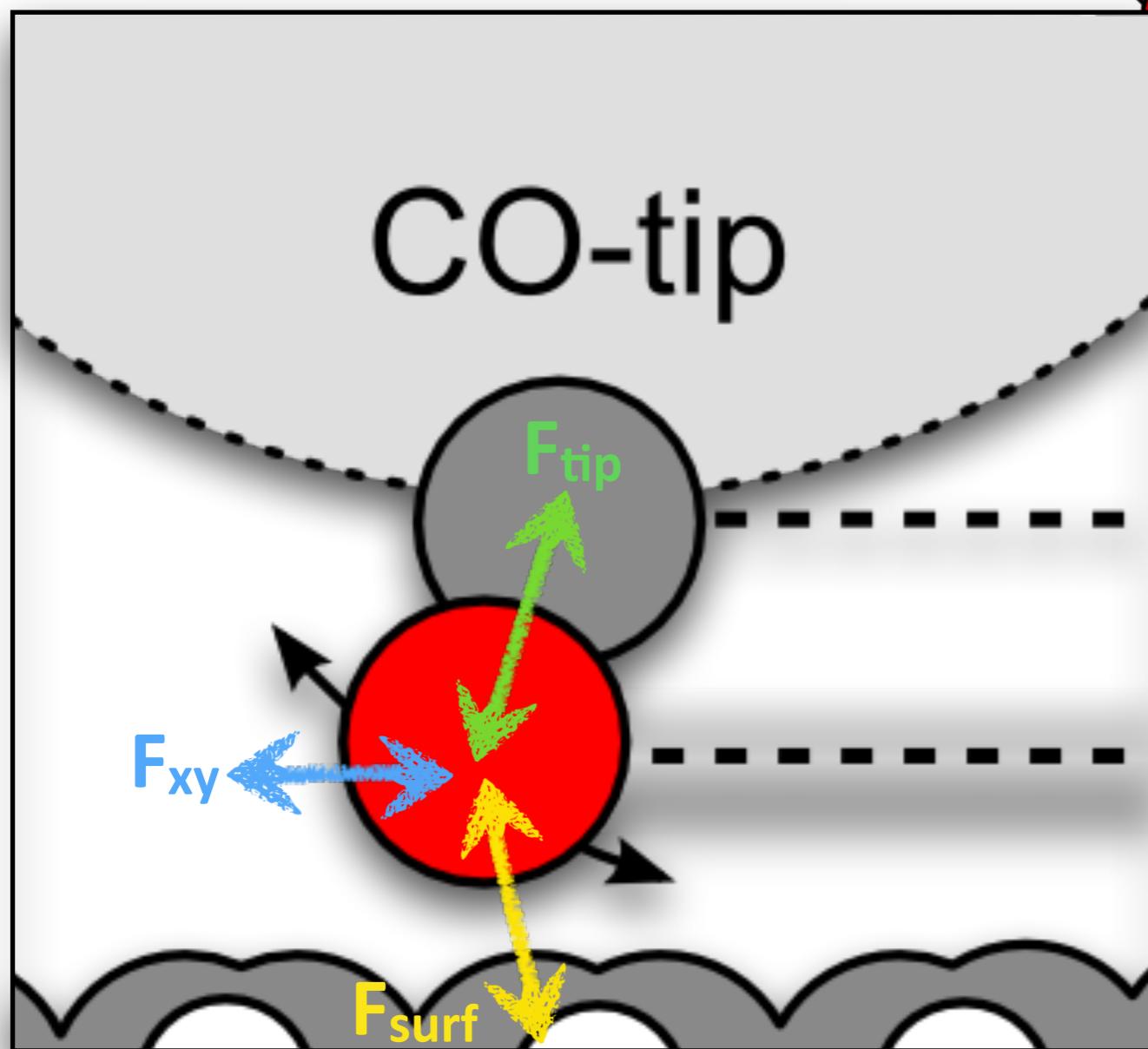
P. Hapala, *et al.*, Phys. Rev. B, 90:085421 (2014)



BORON-GRAPHENE-NANORIBBON vAFM

Mechanical AFM Model

P. Hapala, et al., Phys. Rev. B, 90:085421 (2014)



CO-tip

$z_{control}$

$z_{tip} \pm \Delta z$

0

For every x,y,z minimize:

$$F_{tip} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$

$$F_{xy} = k_{xy} (r_{xy} - r_{0,xy})^2$$

$$F_{surf} = 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r} \right)^{12} - \left(\frac{\sigma_{ij}}{r} \right)^6 \right] + \frac{q_i q_j}{4\pi\epsilon_0\epsilon_R r}$$

Collect F_{surf} and compute Δf

$$\frac{\Delta \omega}{\omega_{res}} = - \frac{1}{\pi a k} \int_{-1}^1 F(z + a(1+u)) \frac{u}{\sqrt{1-u^2}} du$$

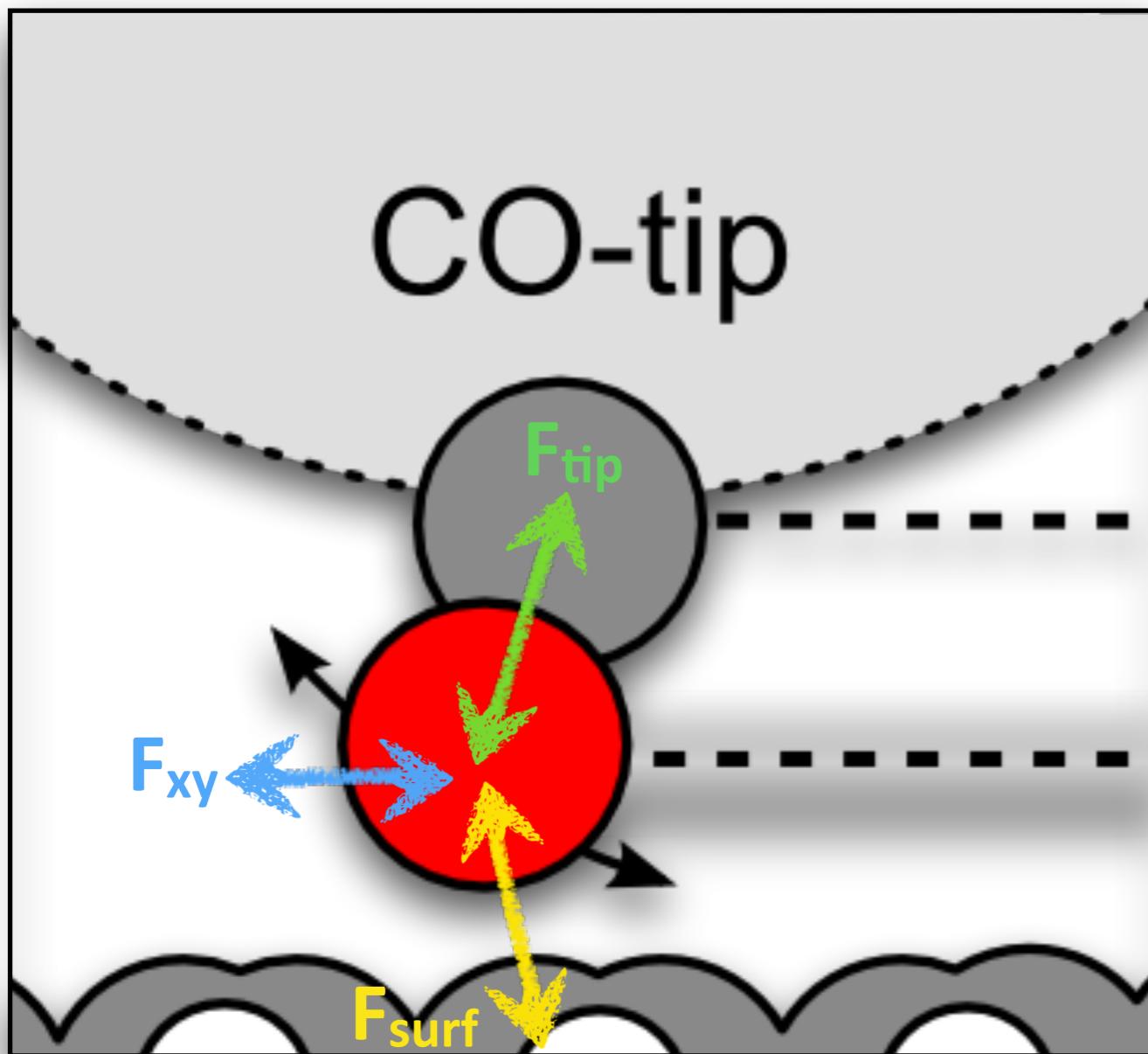
F. Giessibl, Rev. Mod. Phys., 75:949 (2003)

BORON-GRAPHENE-NANORIBBON VAFM

Mechanical AFM Model

P. Hapala, *et al.*, Phys. Rev. B, 90:085421 (2014)

- First: Python implementation
- Too slow: converted to C
- Still too slow: parallel (MPI)
- Now it's pretty fast, :)



```
/* Loop y */
for (iy=0; iy<Npoints.y; ++iy) {
    y = iy*Options.dy; /* Current y */

    /* Check the progress and report every so often */
    n = ix*(Npoints.y+1) + iy;
    if ( (Me == RootProc) && (((double)n)/(nxy)) >= curperc ) {
        debugline(RootProc,"Finished approximately %4.1f %% of the sim
        curperc += checkperc;
    }

    /* Compute on which processor this x,y combination should be run
    onproc = n % NProcessors;
    if (onproc != Me) { continue; }
    PointsOnProc[Me]++;
}

/* Position the tip far above the surface */
Dummy_pos.x = x;
Dummy_pos.y = y;
Dummy_pos.z = Options.zhigh + Options.dz; /* Plus dz to allow for
Tip_pos.x = Dummy_pos.x;
Tip_pos.y = Dummy_pos.y;
Tip_pos.z = Dummy_pos.z - DummyParams.rmin;

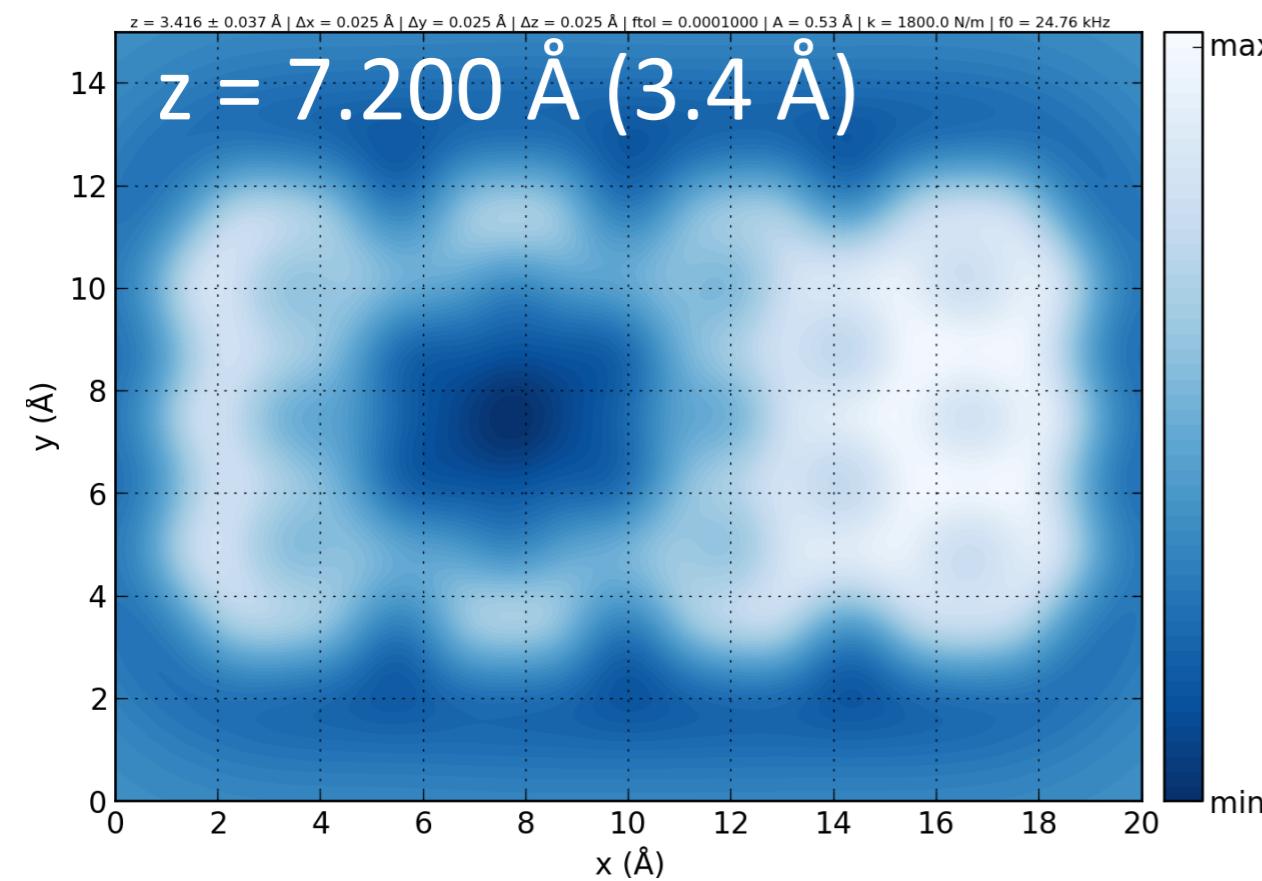
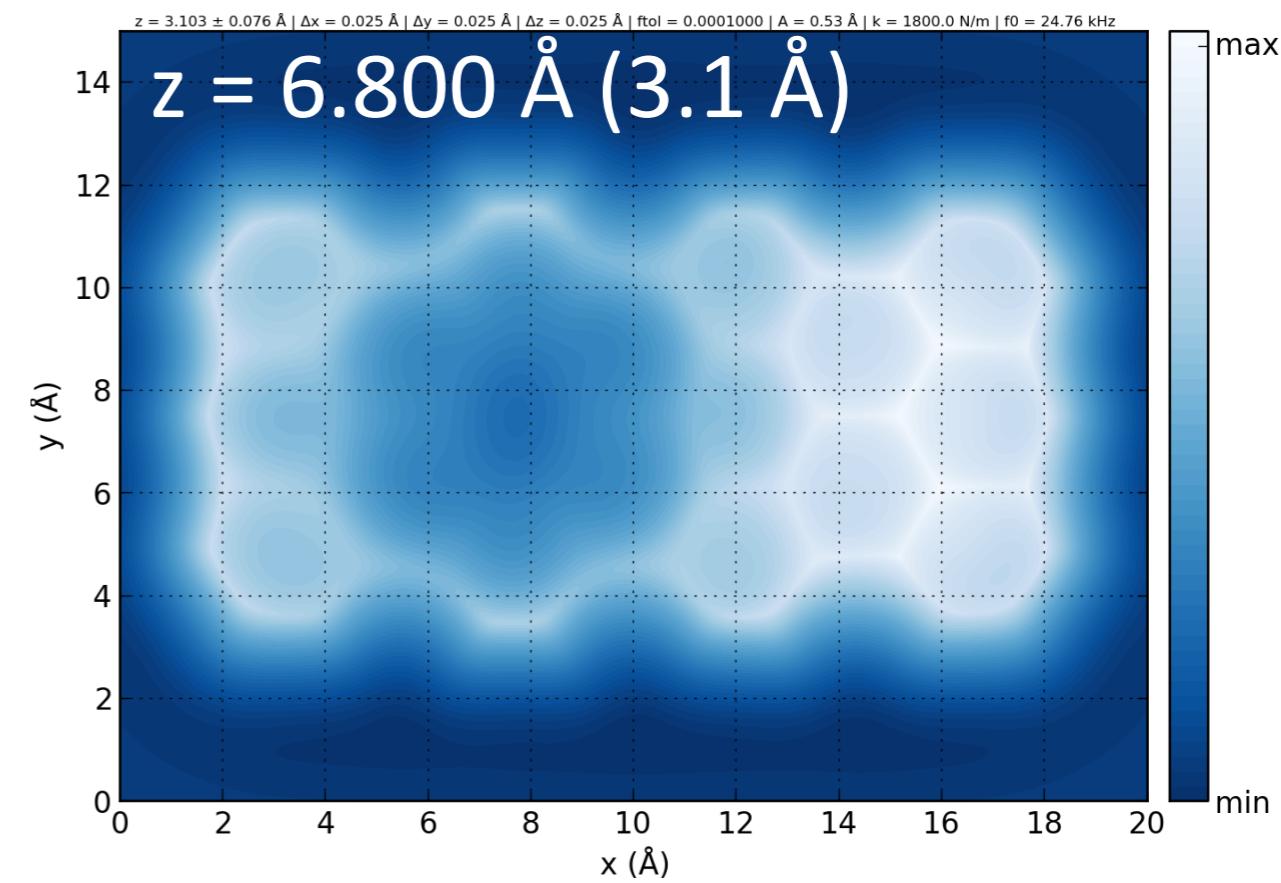
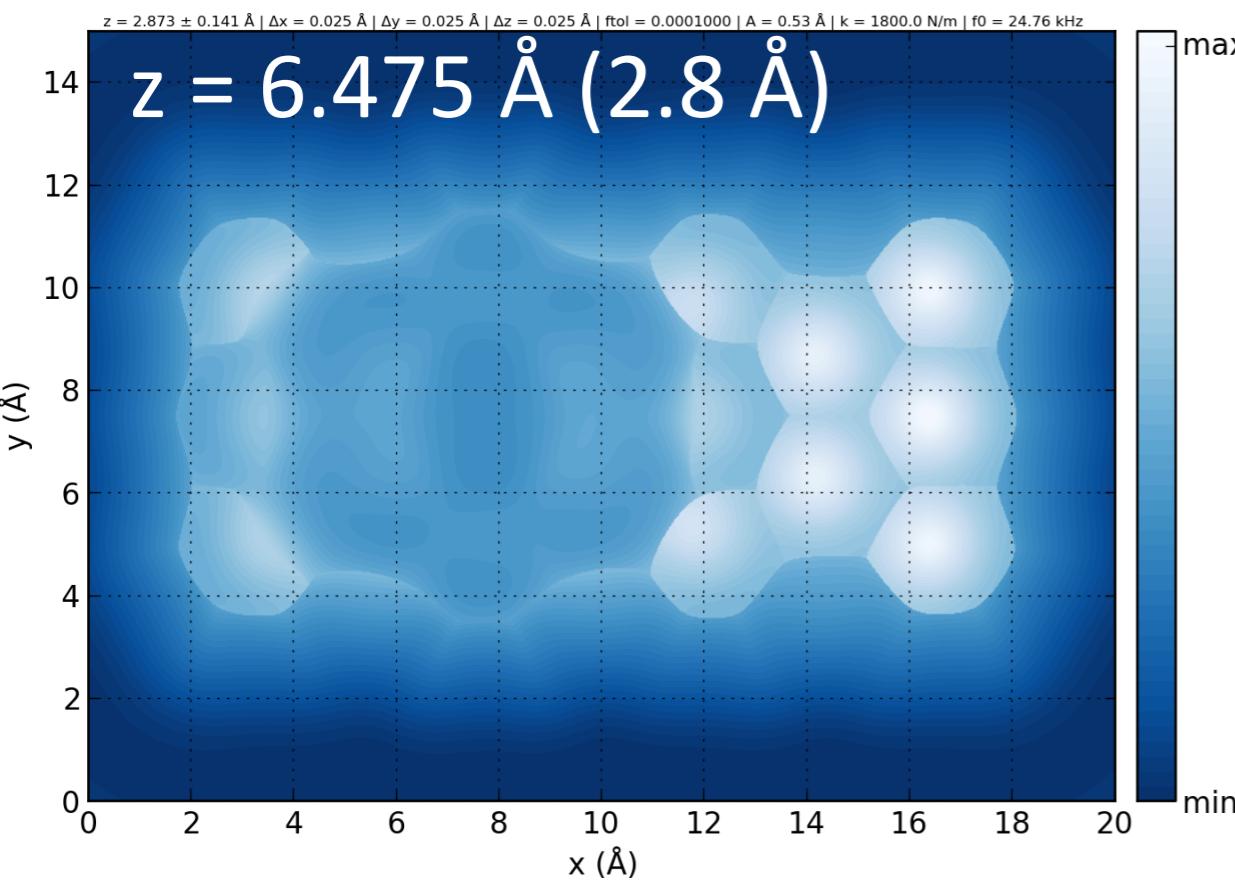
/* Approach and optimize */
nmax = 0;
minangle = 9e99;
maxforce = -9e99;
for (iz=0; iz<Npoints.z; ++iz) {
    z = Options.zhigh - iz*Options.dz; /* Current z */

    /* Move tip and dummy atom toward the surface */
    Dummy_pos.z -= Options.dz;
    Tip_pos.z -= Options.dz;

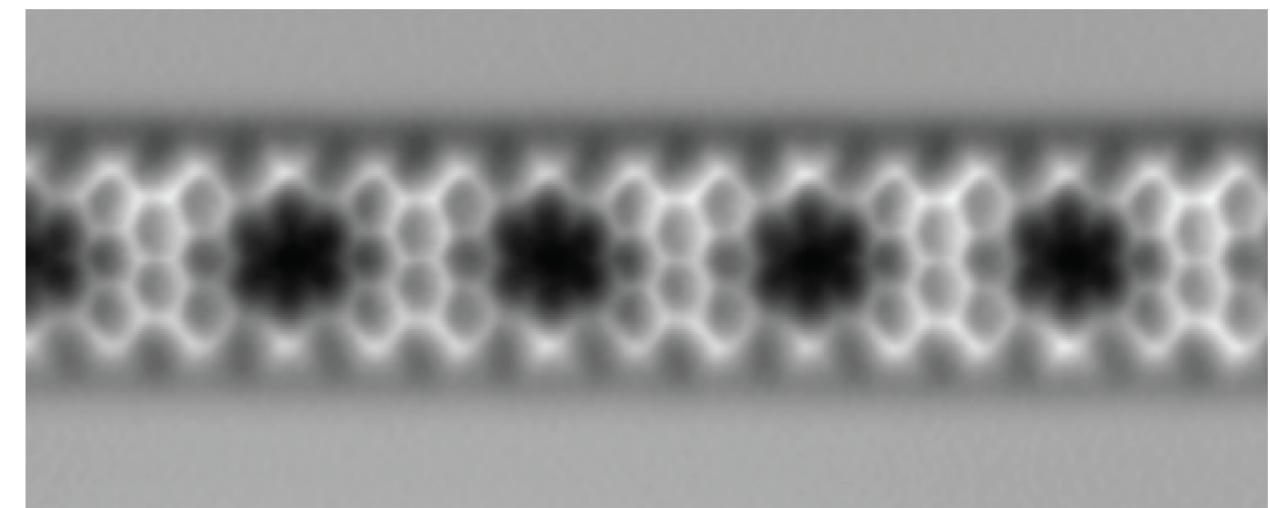
    /* Collect the force */
    ftip[iz] = NULL_vector;
```

68 million positions, 5000 minimizations each, 12 processors → 20 hours

BORON-GRAPHENE-NANORIBBON VAFM

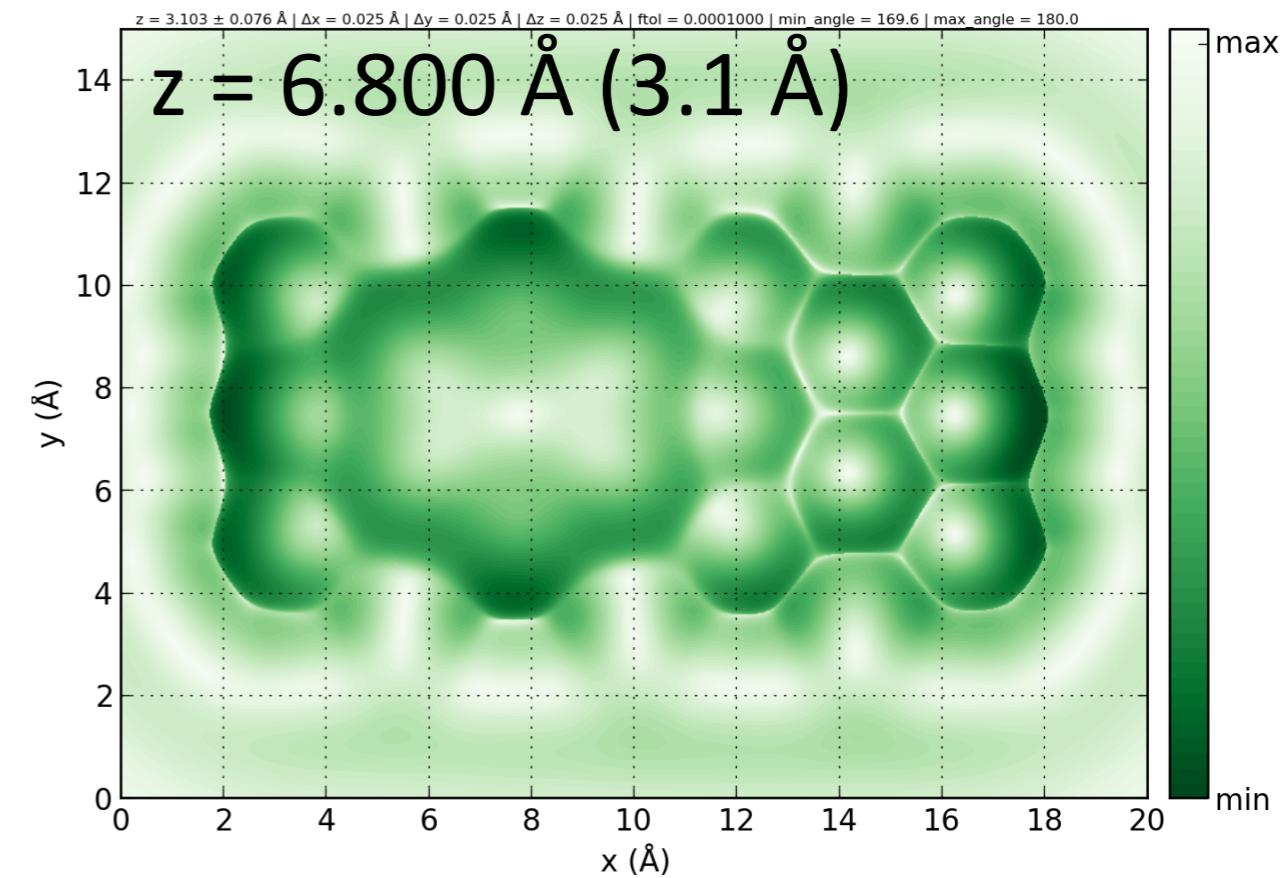
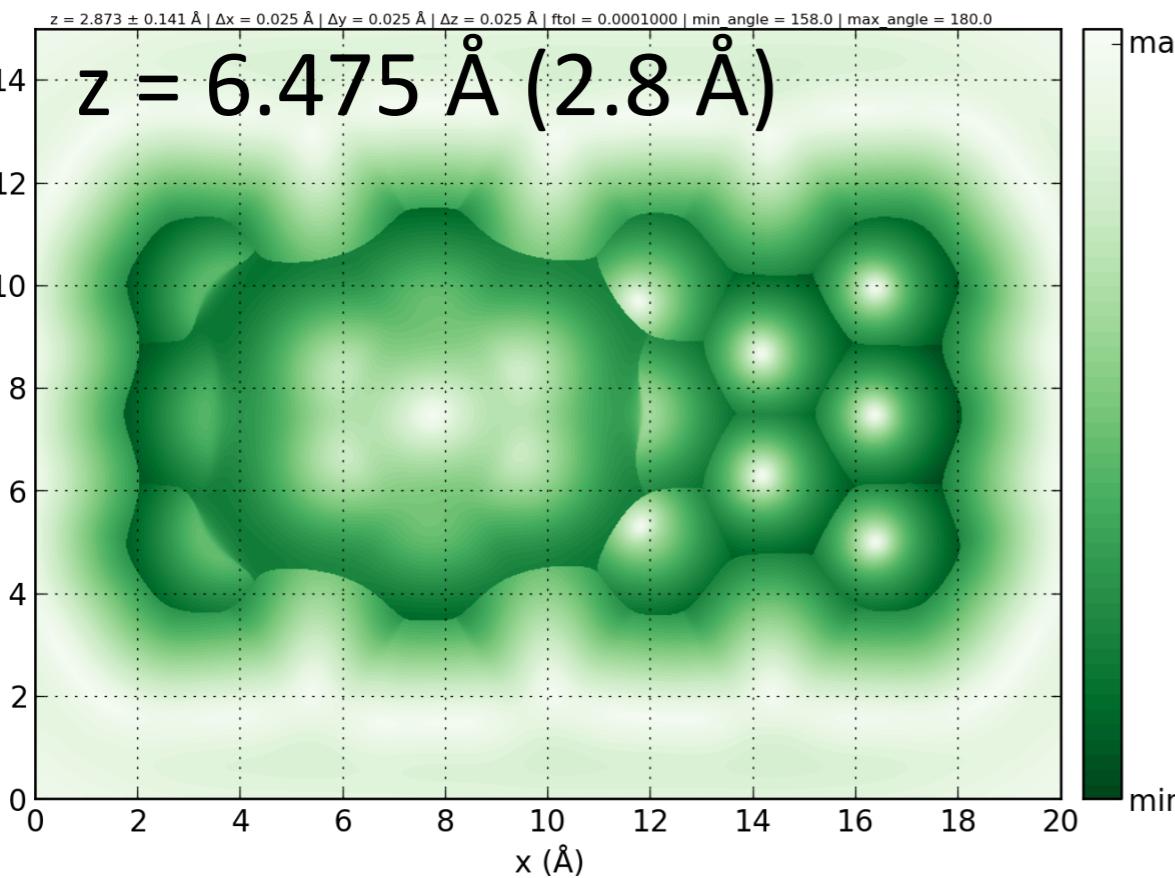


Frequency shift

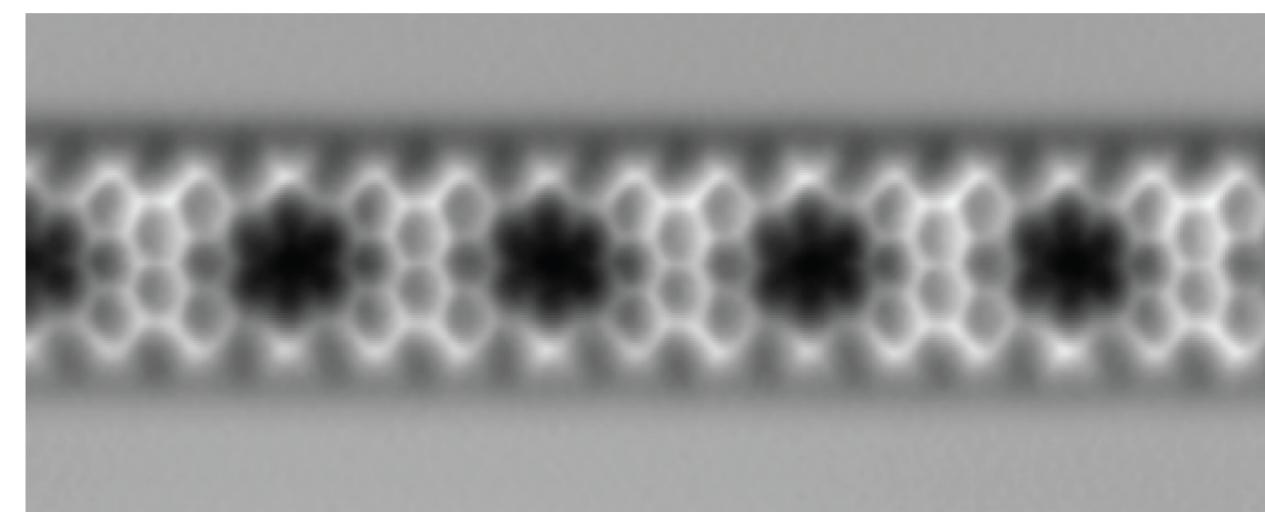
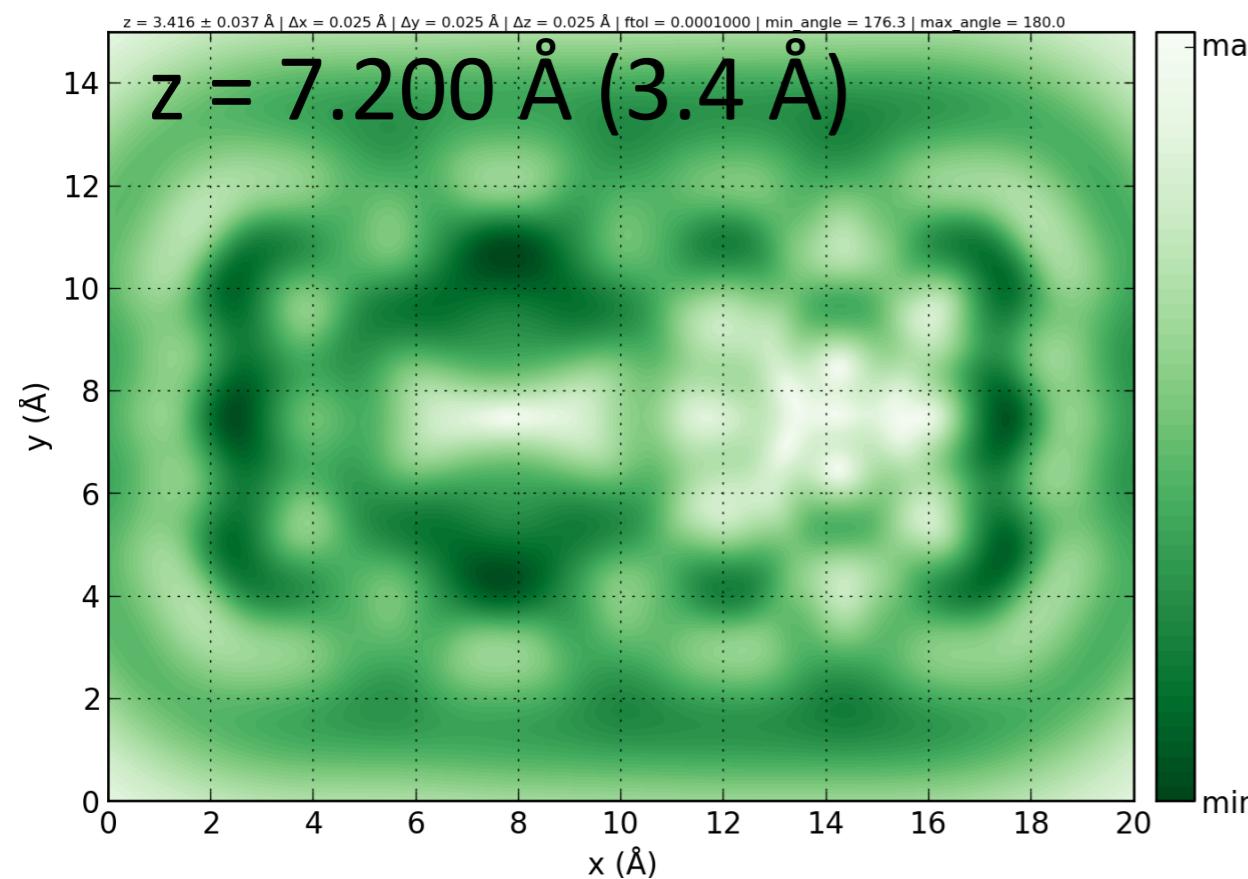


-7.27 -2.57
 Δf (Hz)

BORON-GRAPHENE-NANORIBBON VAFM



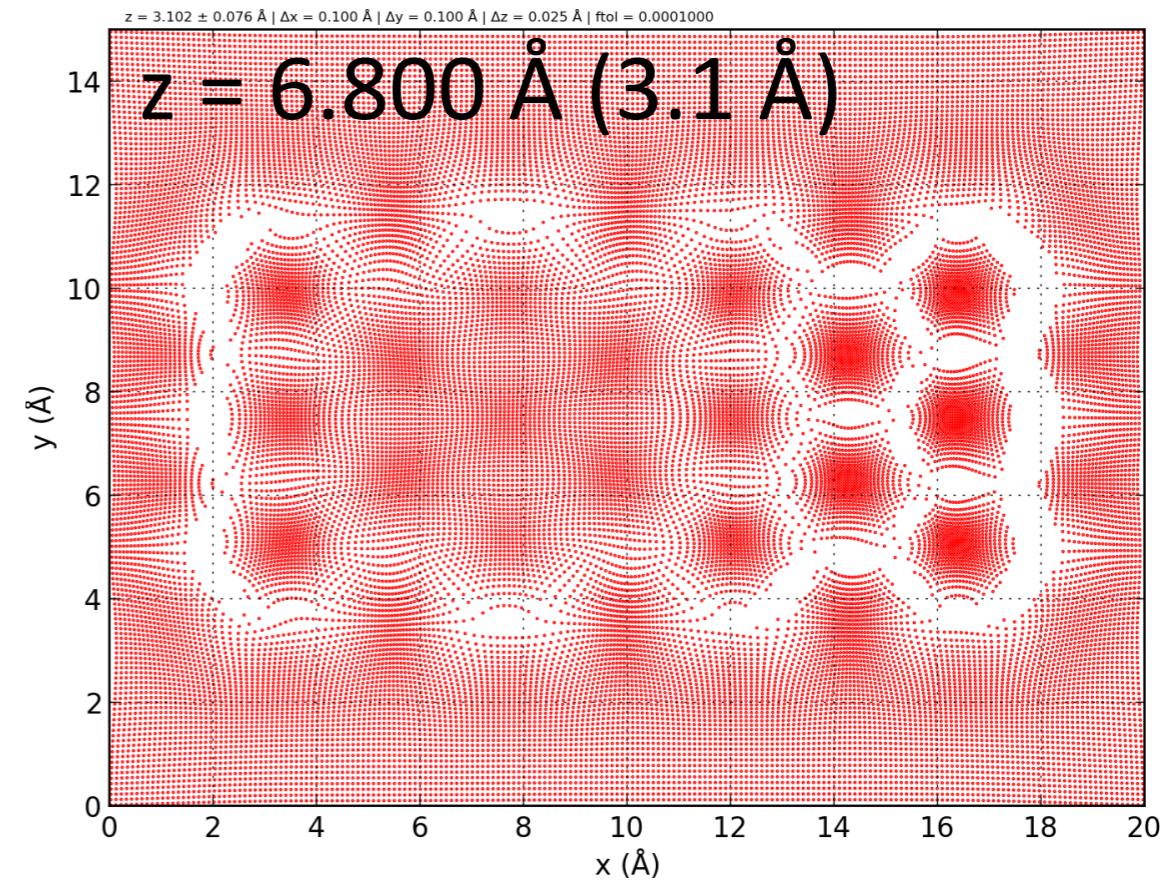
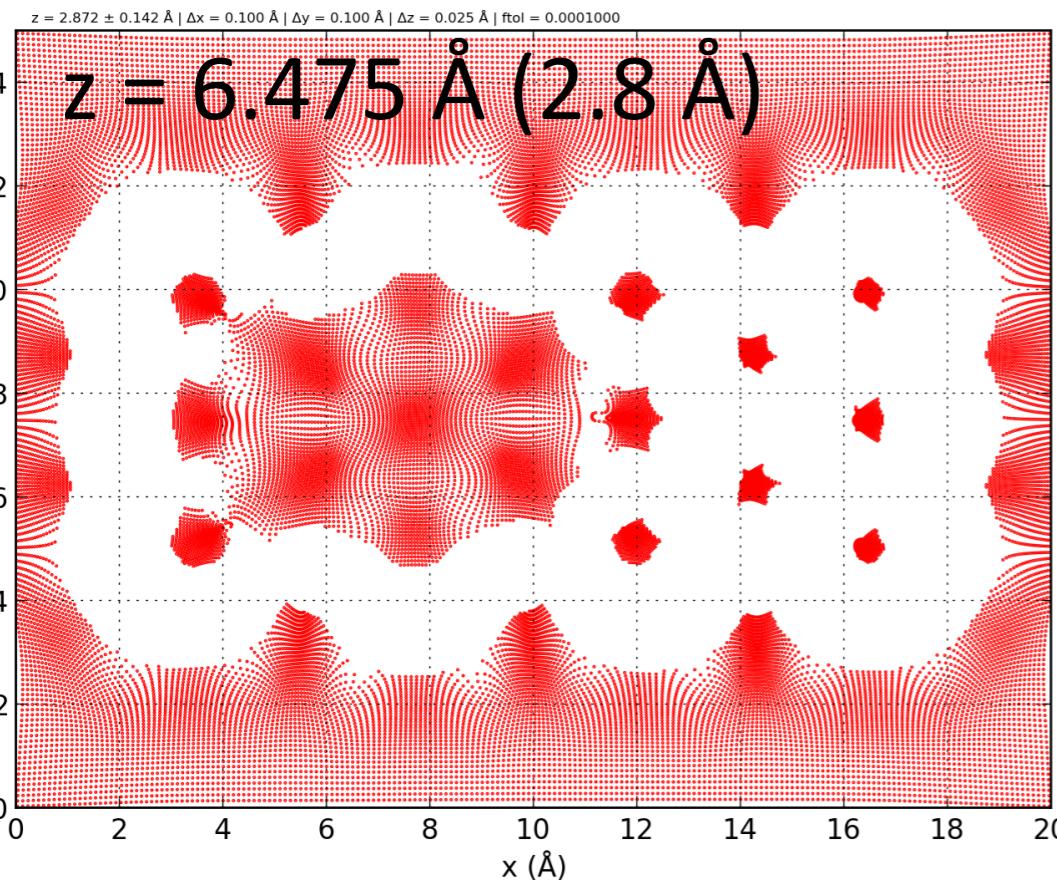
Bending of tip (angle with normal)



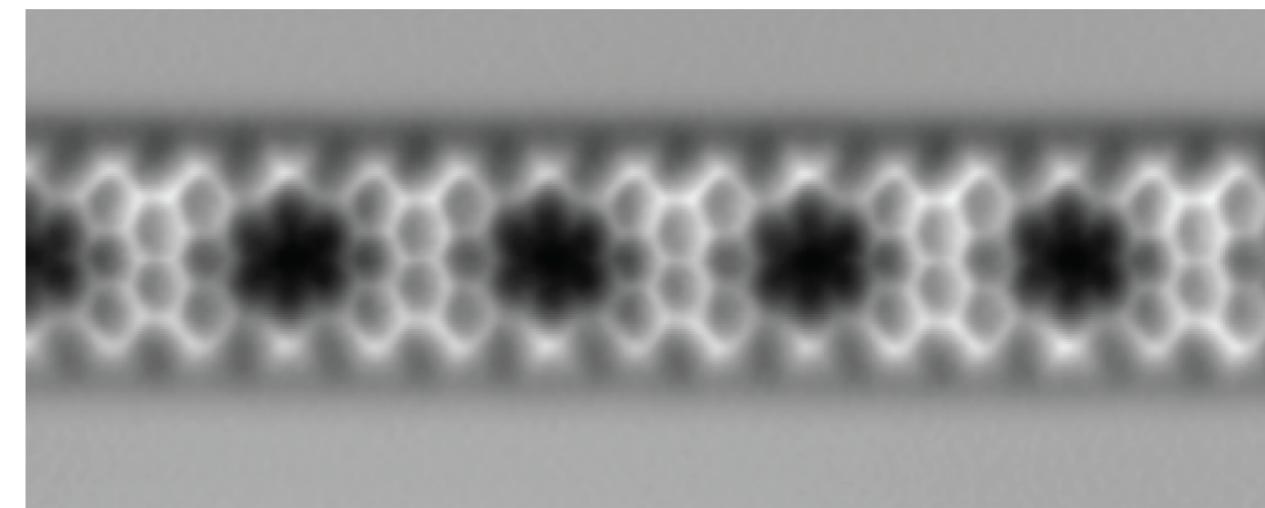
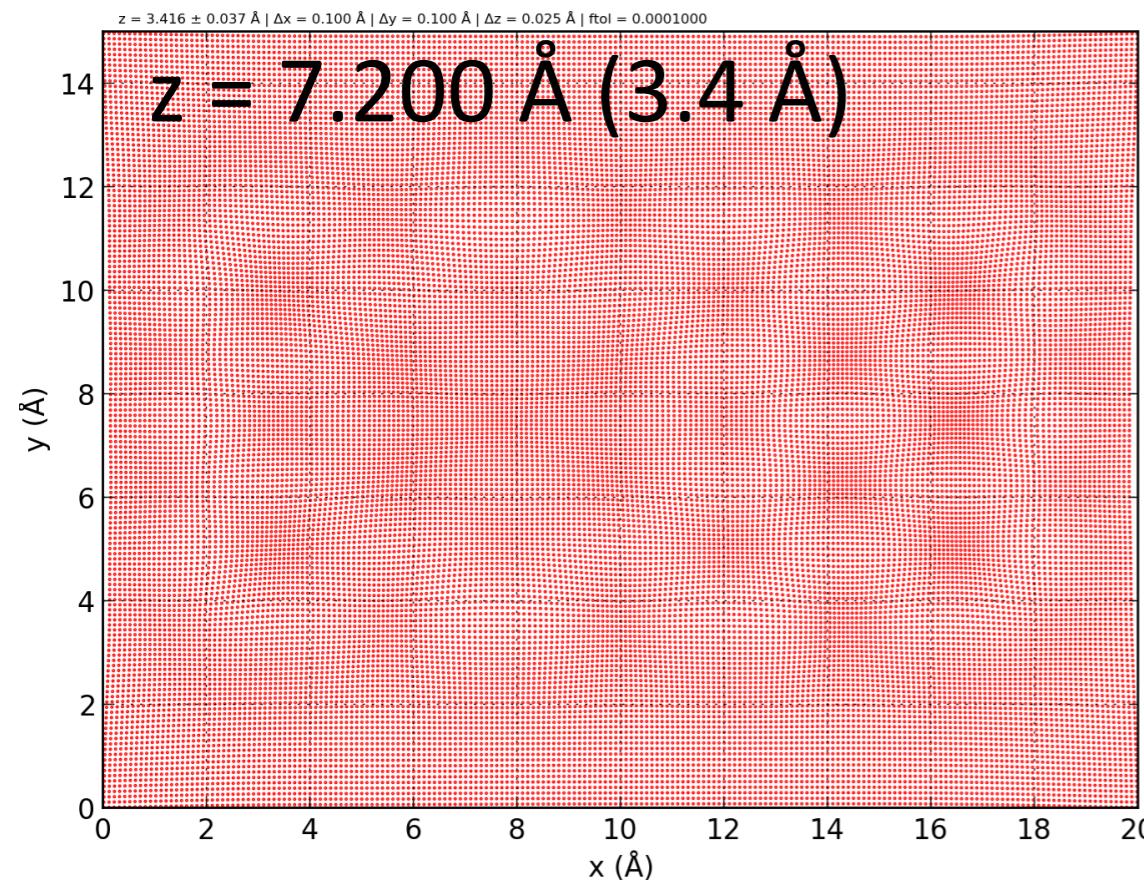
-7.27 -2.57

Δf (Hz)

BORON-GRAPHENE-NANORIBBON VAFM



Displacement of tip (in plane)



-7.27 -2.57
 Δf (Hz)