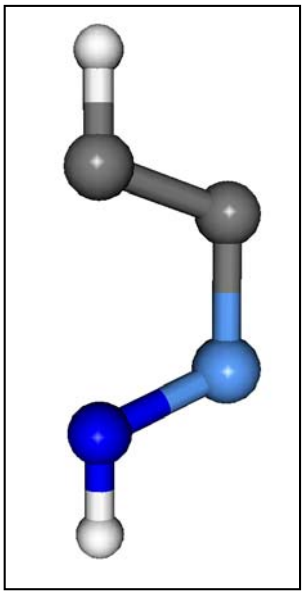
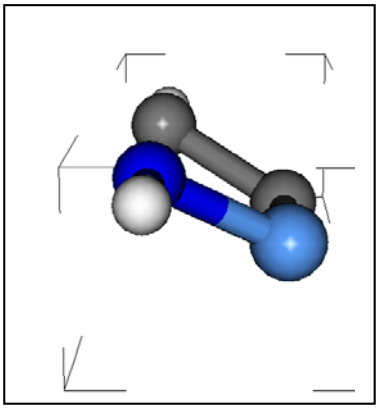
Attached is the input file for the partially hydrogenated (50% on the top and 50% in the bottom) BN-graphene heterosystem. See side and perspective top views for the primitive hexagonal cell (at the left) with *.xyz file for Molekel software (attached). At the right the same structure has been repeated with the colors modified for the publication. The primitive cell contains 2 H (one at each side), 1 B, one N and 2 C atoms. It demonstrates the direct DFT-LDA gap about 1 eV, which might go to 1.6 ÷ 2 eV, which is in a very useful range. The structure is “sufficiently asymmetric” to show SHG.

I understand that this is a short notice (the paper should be submitted on April 20th), but this would be great if the calculation can be done within a week or so. On Mon I have my last lecture this semester, will have finally more time. Let me know if you have any question.





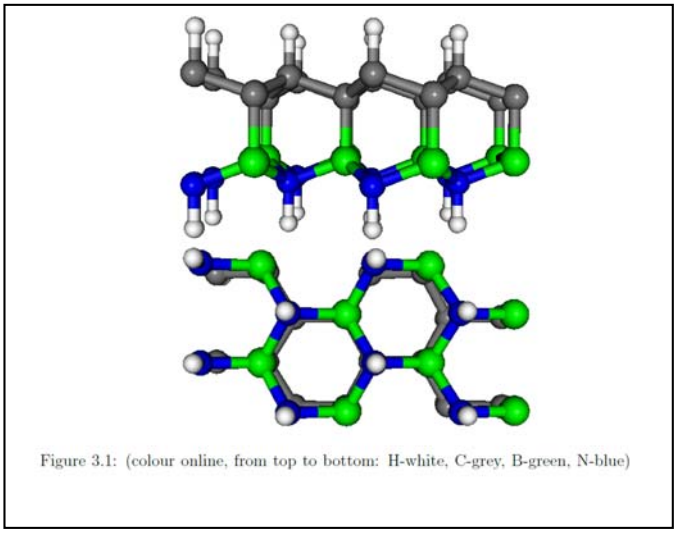


Figure 3.1: (colour online, from top to bottom: H-white, C-grey, B-green, N-blue)

We have many other very interesting structures, we can look at them when I visit Leon, but this
In the fall I go to Germany, Münster, where I want to look at excitonic effects for similar materials.

Please send me also the figures similar to that from PSS, important point, however, is that they should have different format and look differently.

Hexagonal structure

Ibrav = 4 Hexagonal and Trigonal P celldm(3)=c/a