

Optical control of inter-layer distance of hBN: a TDDFT study

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In this presentation, we introduce an idea to modify inter-layer distance of hBN by shining IR laser in resonance with the frequency of the optical phonon (A_{2u} mode). By performing the TDDFT-MD simulation under the IR laser, significant growth in the amplitude of the A_{2u} phonon mode was observed and inter-layer contraction over 11% of the original distance was achieved. The source of the stronger attraction of hBN sheets was attributed to the increase of dipole moment of each layer coming from the motions of boron (B) and nitrogen (N) atoms in opposite directions. Since the dipole moments of these layers remain parallel throughout the A_{2u} phonon vibration, the increase of attractive force occurs between the two hBN sheets in analogy of the London force. In this talk, we will further discuss the proper intensity of IR laser and potential applications of this phenomenon. This work was published in *Phys. Rev. Lett.* **114**, 116102 (2015).