

Abstract Submitted
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Optical control of inter-layer distance of hBN: a TDDFT study
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HIDE MIYAZAKI, AIST, ANGEL RUBIO, Max Planck Institute for the Structure
and Dynamics of Matter — 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 grow in an amplitude of the A_{2u} phonon mode was ob-
served and inter-layer contraction over 11 % of the original distance was achieved.
The source of the stronger attraction of hBN sheets was attributed with 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
as 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 proper intensity of IR laser and potential applications of this
phenomenon. This work was published in Phys. Rev. Lett **114**, 116102 (2015).

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