Photo-Enhancement of Cohesion;
Cases of Noble Atoms and Layered Materials

Yoshiyuki Miyamoto*, Hong Zhang**, Takehide Miyazaki* and Angel Rubio[†,‡]
** Nanosystem Research Institute, National Institute of Advanced Science and Technology (AIST), Japan*
E-mail: yoshi-miyamoto@aist.go.jp
*** College of Physical Science and Technology, Sichuan University, China*
[†]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany,
[‡] Universidad del País Vasco, Spain

This presentation shows our theoretical prosal of photo-enhancement of weak cohesion in noble gases and layered materials. Our idea stands for London's mechanisms of the van der Wassls forces, namely dynamical dipole-dipole attraction. We found that light near the resonance of either electronic or vibronic excitation can enhace the dipole moment. We have tested two simple systems, the first is a dimer of helium (He) atoms and the other is bi-layer of hexagonal boron-nitride (hBN).

In case of He dimer, we performed simulation with extreme ultra-voilet light that is very close to He 1s →2p excitation energy. When the polarization vector of the light is parallel to He-He axis, the light induce oscillation of electron cloud which causes parallel dipole moment on each He atom. Due to a concerted motion of electrons and nuclei, the He atoms are accerated to shorten their distance. The estimated photo-induced effective force is over 7 pN[1]. Meanwhile, in case of hBN, we found that infrared light can induce out-of-plane optical phonon, A_{2u} mode, which produces parallel dipole moments to attract each layer. Depdenting on the intensity of light, the speed of inter-layer contraction is governed. Subsequent electronic excitation was also exmianed under high intensity of light.

The present simulations were performed within the time-dependent density functional theory[2], using the plane-wave code[3] with alternating scalar potential mimicking optical field that satisfies total-energy conservation rule[4] within adiavatic exchange correlation functional. All calculations were performed by using AIST-super cloud generation II. YM acknowledges support from a fund from the Science of Atomic Layers (SATL), and the Computational Materials Science Initiative (CMSI), runned by MEXT.

1. Y. Miyamoto, T. Miyazaki, A. Rubio, and H. Zhang, Appl. Phys. Lett. **104**, 201107 (2014).
2. E. Runge and E. K. U. Gross, Phys. Rev. Lett. 52, **997** (1984).
3. O. Sugino and Y. Miyamoto, Phys. Rev. B**59**, 2579 (1999); B**66**, 089901(E) (2001).
4. Y. Miyamoto and H. Zhang, Phys. Rev. B77, 165123 (2008).