

Carbon Nanotube as a Laser-Field Amplifier for Efficient Water Decomposition: A TDDFT Study

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In former work, we have investigated laser-field enhancement on 2D graphitic sheets by performing the TDDFT-MD simulation under alternating electric field (E-field). We found over 120 % enhancement of laser field which helps laser-induced water decomposition with lower threshold intensity. On the other hand, with use of carbon nanotube (CNT), the enhancement has become twice that reduced the threshold power of decomposition as a quarter of that needed for isolated water decomposition. We have performed TDDFT MD simulation using triple period of (8,0) semiconducting CNT containing 15 water molecules, which were initially placed randomly. The assumed laser field has wavelength 800nm and full-width of half-maximum (FWHM) 10 fs for optical field intensity. With shorter optical field 400nm, the threshold intensity was further reduced. The figure below shows decomposition of part of water molecules (pink colored ones) with wavelength 800nm, FWHM=10fs.

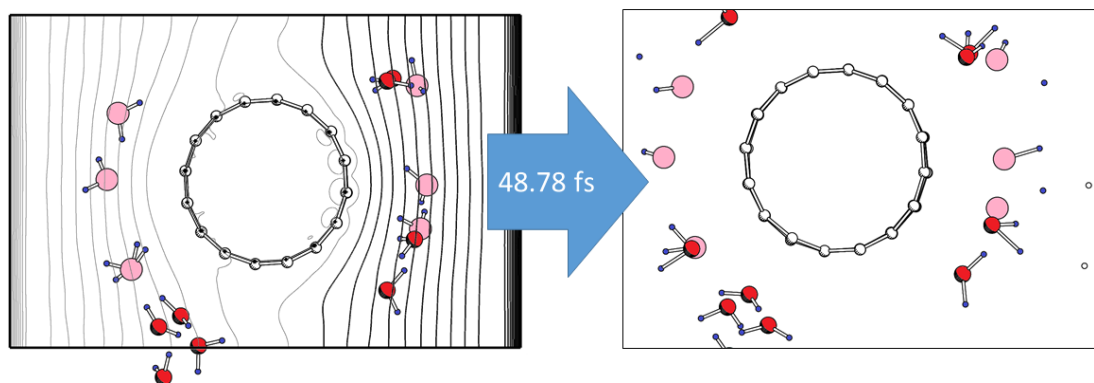


Fig. 1: (Left) Snapshot of 15 H₂O molecules around CNT and optical field distribution, and (Right) decomposition of water with pink colored balls. The views along with CNT axis are shown.

In this poster presentation, I will discuss physics behind this phenomena and practical applications. This work was financially supported JSPS KAKENHI, with grant numbers JP16H00925, JP16K05049, JP16K05412, and JP16H04103

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