Enhanced Laser Field by Planar and Curved Graphitic Materials Applied for Water Decomposition: A TDDFT Study

Yoshiyuki Miyamoto[1,*], Hong Zhang[2], Xinlu Cheng[3], Angel Rubio[4,5]

[1]National Institute of Advanced Industrial Science & Technology (AIST), Central 2, 1-1-1, Umezono, Tsukuba, 305-8568, Japan, [2]College of Physical Science & Technology, Sichuan University, Chengdu 610065, China, [3]Key Laboratory of High Energy Density Physics and Technology of Ministry of Education, Sichuan University, Chengdu 610064, China, [4]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany, [5]Nano-Bio Spectroscopy Group and ETSF, Universidad del País Vasco, CFM CSIC-UPV/EHU-MPC, 20018 San Sebastián, Spain

Corresponding author(s): yoshi-miyamoto@aist.go.jp

Strong and short pulse laser is applied as manufacturing tools. Currently available laser equipment can decompose water molecules that opens a way to producing hydrogen fuel alternative to conventional fossil fuel. By performing the time-dependent density functional theory (TDDFT) simulation, we propose that the necessary laser power for water decomposition is reduced by using 2-dimensional sheets and tubule form of graphitic materials. By assuming the full-width-of-half-maximum 10fs for wavelength 800 nm, we have studied decomposition of a water molecule being isolated or being located near 2-dimensional sheets or carbon nanotubes. The computed power threshold for water decomposition can be reduced by factor 2 by using the 2-dimensional sheet, and by factor 4 by using the carbon nanotubes compared to the power for decomposing pure water.

By computing the modulated optical field by TDDFT calculation, field enhancement near 2D sheet [1] as well as near carbon nanotube [2] was observed that is consistent with factor of threshold power reduction for water decomposition. The cause of reduction is optical field enhancement near 2 dimensional sheet as well as carbon nanotube. Especially for carbon nanotube, the field enhancement is not only coming from polarization but also by curvature of the wall of the tube that helps field concentration [2].

Figure 1 demonstrates present TDDFT-MD simulation of mono-layer water molecules above graphene sheet tested for the three different initial atomic configurations that give the same threshold power for the decomposition. Practical estimation of yield of water decomposition compared to the reported value obtained by using photo-catalysis with ordinary light will be discussed.

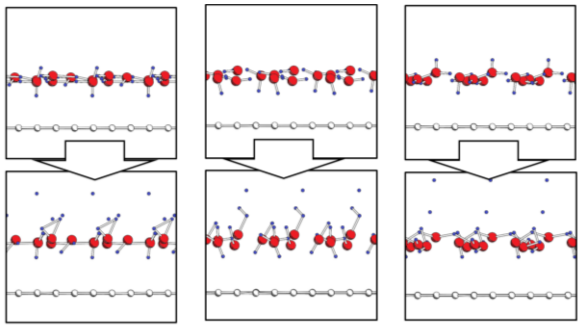

Fig.1 Snapshot of decomposition for one mono layer water molecules above graphene sheet. Three different initial atomic configurations were tested giving the same power threshold of the decomposition.

[1] Y. Miyamoto, H. Zhang, X. Cheng, and A. Rubio, Phys. Rev. B **96**, 115451 (2017).

[2] Y. Miyamoto, H. Zhang, X. Cheng and A. Rubio, *under preparation*.