Nanotubes as laser-field enhancer useful for water decomposition: A TDDFT study

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By performing the real-time TDDFT calculation coupled with classical molecular dynamics, we studied laser-field induced water decomposition near the carbon nanotubes. Short and intense laser field can provide high photon flux which is useful for high yield of photo-chemical reaction such as water decomposition harvesting hydrogen fuel. One demanded technology is to reduce laser power necessary for water decomposition with aid of some material that enhances laser field intensity. In case of short laser pulse with full-width-of-half-maximum 10 fs, the presence of (8,0) nanotube is found to significantly reduce threshold laser power needed for water decomposition. When laser wavelength is 800 nm, the factor of the power-reduction is less than quarter while the amount becomes less than one eighth with wavelength of 400 nm. Since carbon nanotube is durable upon laser shot, we expect repeat of laser shining for cyclic water decomposition. We discuss physics of laser field enhancement which can be polarization and curvature effect of carbon nanotube.