

---

**The Excited State Dynamics Driven by Ultrafast Laser: Applications of TDDFT and Non-Linear Phononics**

---

Professor ZHANG Hong (张红), Sichuan University, China

---



Professor ZHANG Hong is a full professor in College of Physics, Sichuan University, China. She received her PhD from Sichuan University. Her research area is Condensed Matter Theory and now the research activity is focused on the interaction between short-pulse laser and surfaces (including nanotubes and graphene); hydrogen storage. Her research highlight is targeting high-melting low-dimensional material such as graphene and carbon nanotubes, these materials are experimentally studied and because of their high melting temperatures, heat treatment that control defects, impurities, even entire shape of these material are difficult that make these materials hard to be used for many applications. She is searching non-thermal way to control these materials with use of femtosecond laser. Professor ZHANG has published over 200 publications in PNAS; Physical Review Letters; Physical Review B; Applied Physics Letters and other scientific journals.

---

**Abstract:**

Strong and short pulse laser is applied as manufacturing tools. By performing the time-dependent density functional theory (TDDFT) calculation coupled with classical molecular dynamics, we studied laser-field induced new characteristics of nano functional materials. 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.

In this talk, I will present the applications of photo-chemical reaction by using femtosecond lase and non-thermal process for new material phase. The dynamic behaviour of the light-induced magnetization of MnF<sub>2</sub> introduced through the non-linear phonon-phonon interaction was discussed.

**References**

- [1] H. Zhang\*, et al, Applied Physics Letters, 111, 253303, 2017, Detection of coherent electron dynamics in benzene and polycyclic benzene by two anti-phase pulses: An ab initio study.
- [2] Y. Miyamoto, H. Zhang\*, et al, Physical Review Letters, 114, 116102, 2015 Modifying the interlayer interaction in layered materials with an intense infrared laser
- [3] Y.Miyamoto, H. Zhang\*, XL Cheng, and A. Rubio, Physical Review B, 99, 165424, 2019, Abinitiosimulation of laser induced water decomposition close to carbon nanotubes
- [4] Y. Kong, H. Zhang, et al, Physica B 620,413248, 2021, Regulation of Nb<sup>3+</sup>, Sb<sup>3+</sup> and V<sup>3+</sup> doping on the photo-induced ferroelectricity of KTaO<sub>3</sub>.
- [5] R. Tang, H. Zhang\*, et al, Physical Review B (submitted), The ultrafast magnetization dynamics in light-driven MnF<sub>2</sub>.