Energy Material Research in Soft X-ray

Sang Han Park

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XAS/XES endstation – solid sample

XFEL properties

- Energy range : 0.28 keV ~ 1.2 keV
- Mono energy resolution (E/ ΔE) : 5000 ~ 10000
- Focus size ~ 50 x 50 μm (H x V)

sample environment

- Sample Temperature : 15 ~ 400 K
- Sample DOF : 6 axis [(x, y, z), (Θ,χ,Φ)]
- UHV sample load lock system
- Electron or fluorescence XAS using MCP detector

❖ **Catalyst materials**

Metal oxides: TiO_2, CeO_2, Fe_2O_3, $CuFe_2O_4$

organic materials : N-graphene, $Rebpy(CO)_3Cl$

To identify :

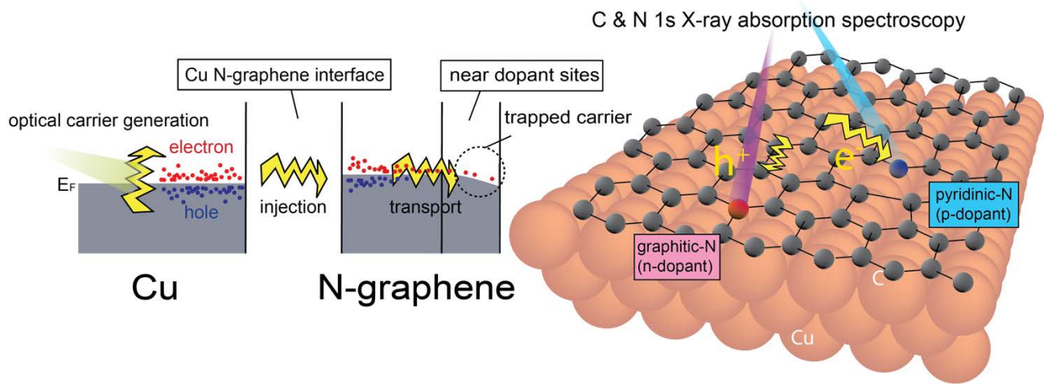
carrier dynamics

charge transfer dynamics

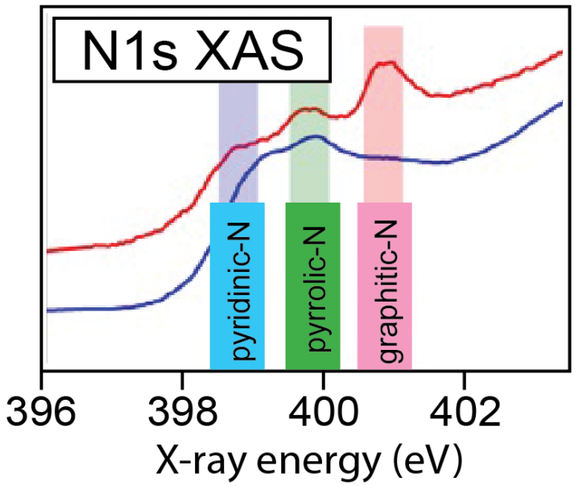
catalytic active site

initial reaction step

N-graphene

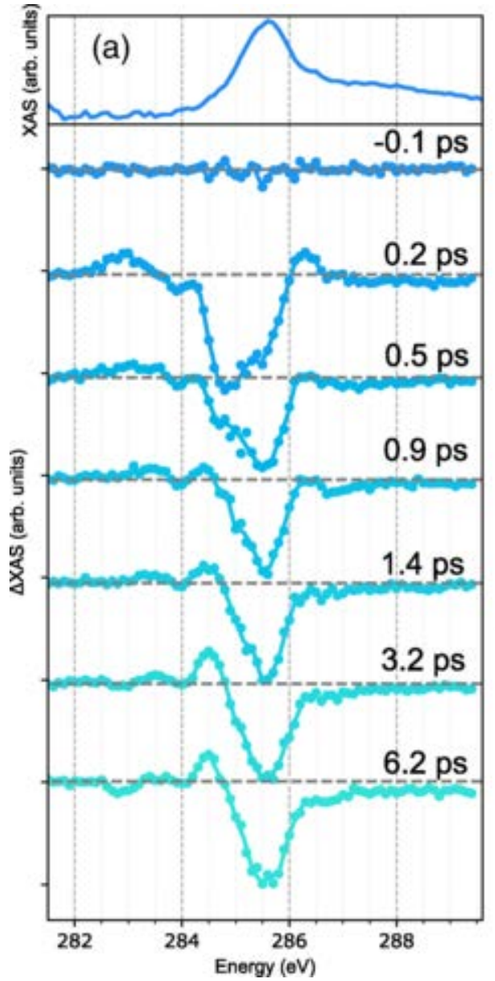


Expected charge transfer from Cu to N



Identifying
charge transfer character
for each N-bonding

XAS of graphene at C K-edge



e-h pair and
e transfer from Cu

e-h recombination

Thermally induced
structural deformation

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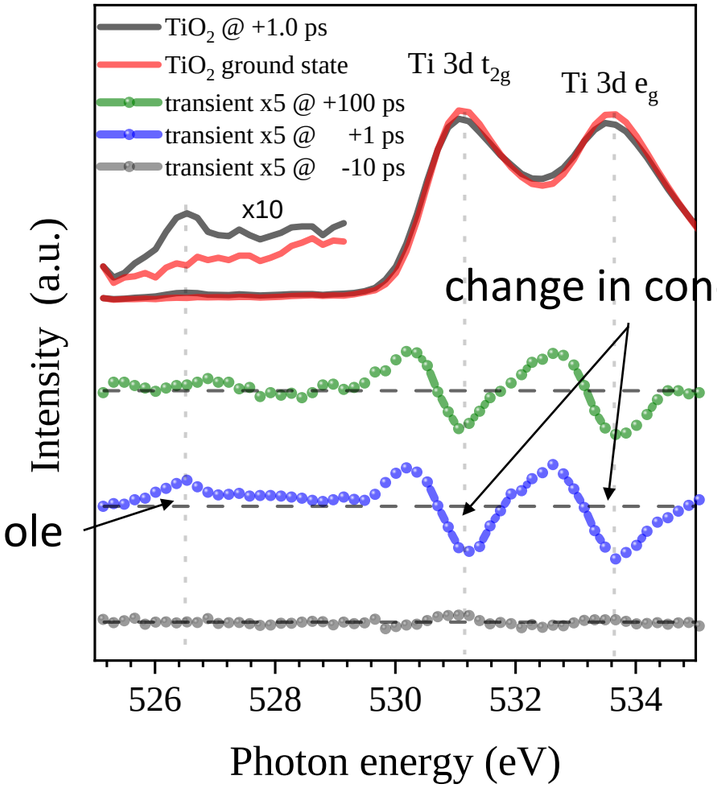
TiO_2 : Dynamics of photo-excited electron and hole

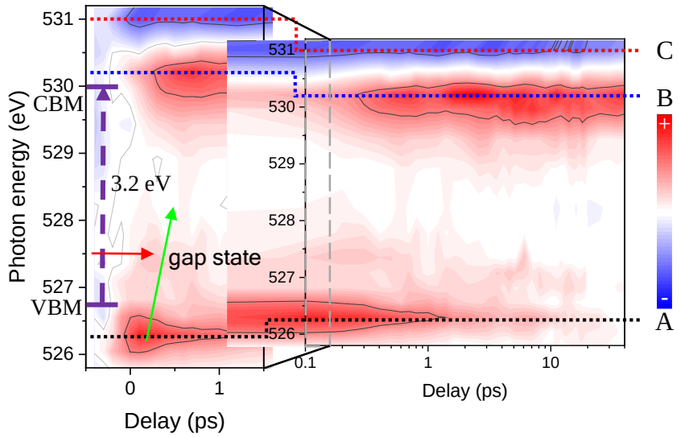
photocatalytic water splitting material : TiO_2

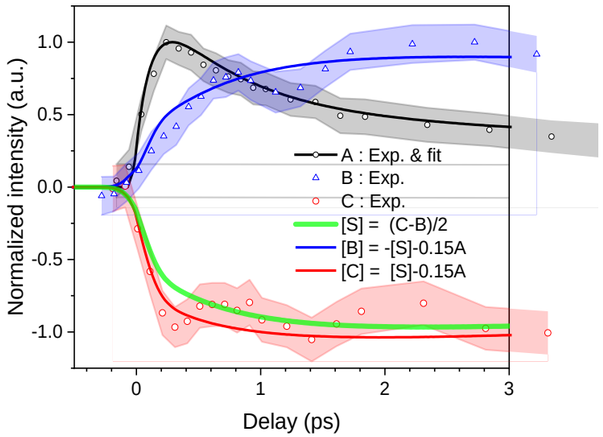
XAS of TiO_2 at O K-edge



change in conduction band

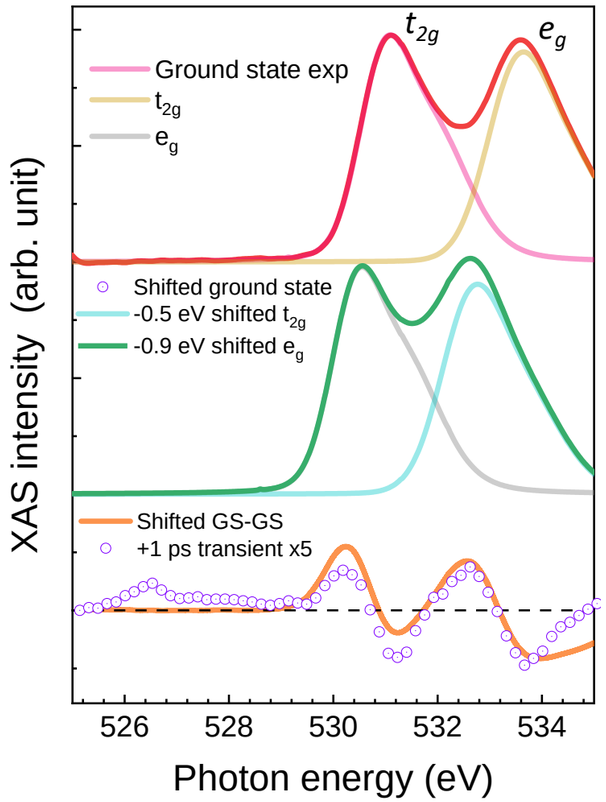
photo-generated hole

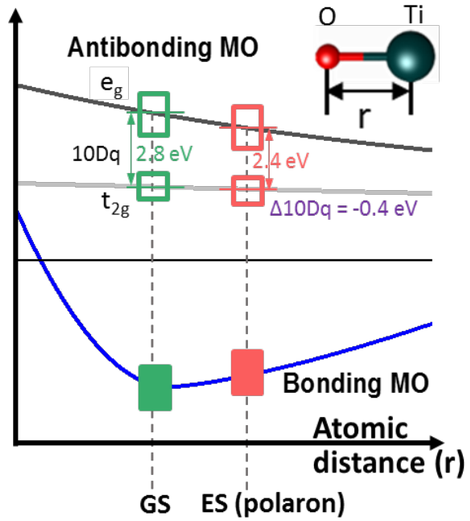


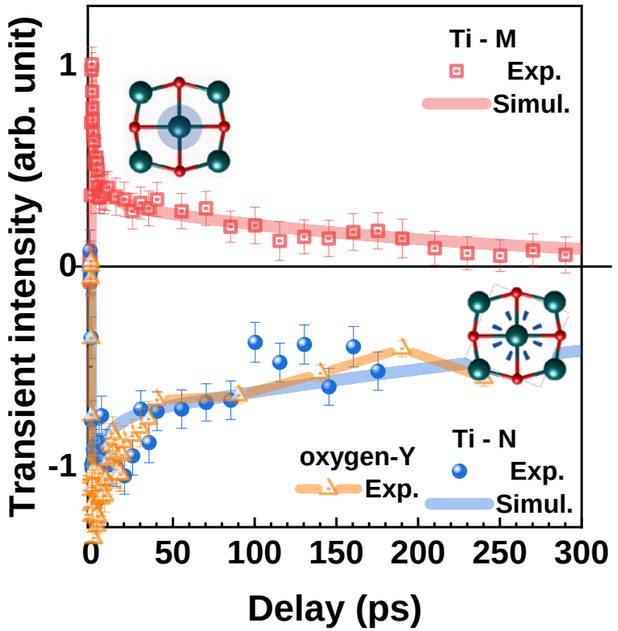


TiO_2 : Dynamics of photo-excited electron and hole

change in conduction band represent increase in bonding length



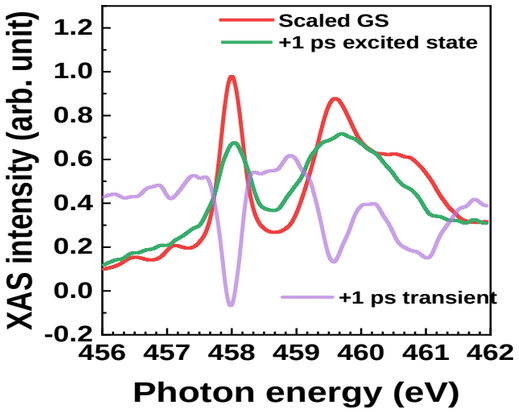


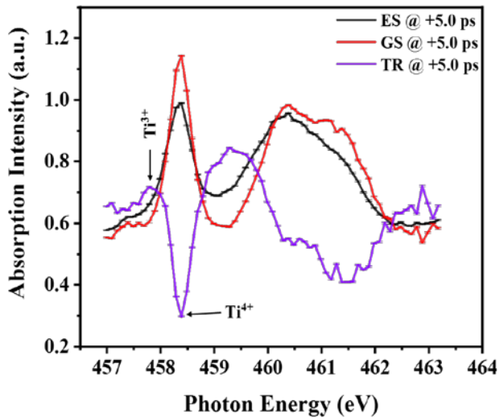


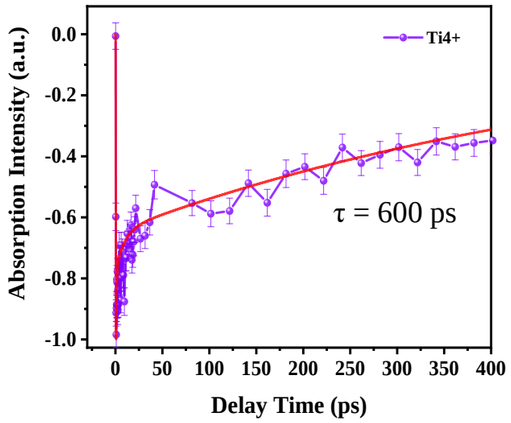
charge localization-> structural change-> charge delocalization -> structure recovery

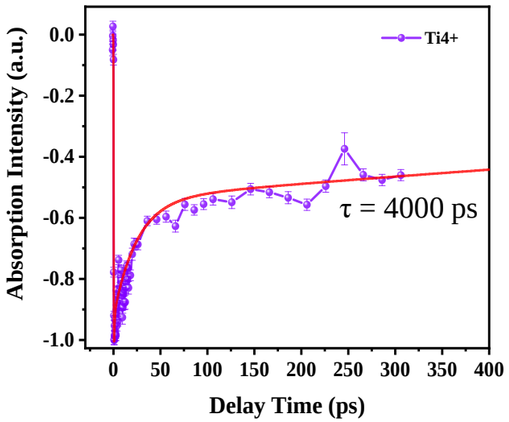
TiO_2 : solid and liquid

comparison of dynamics between solid and solution phase





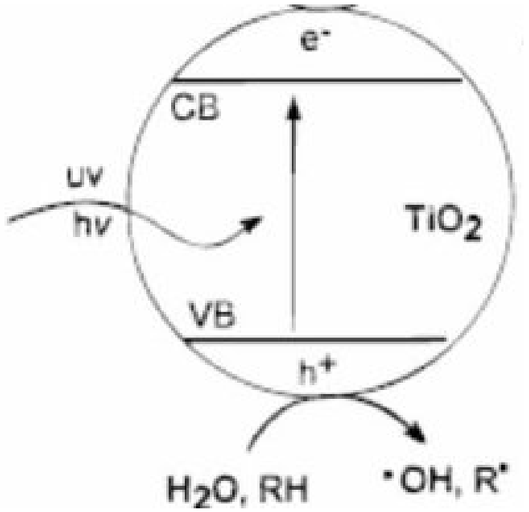




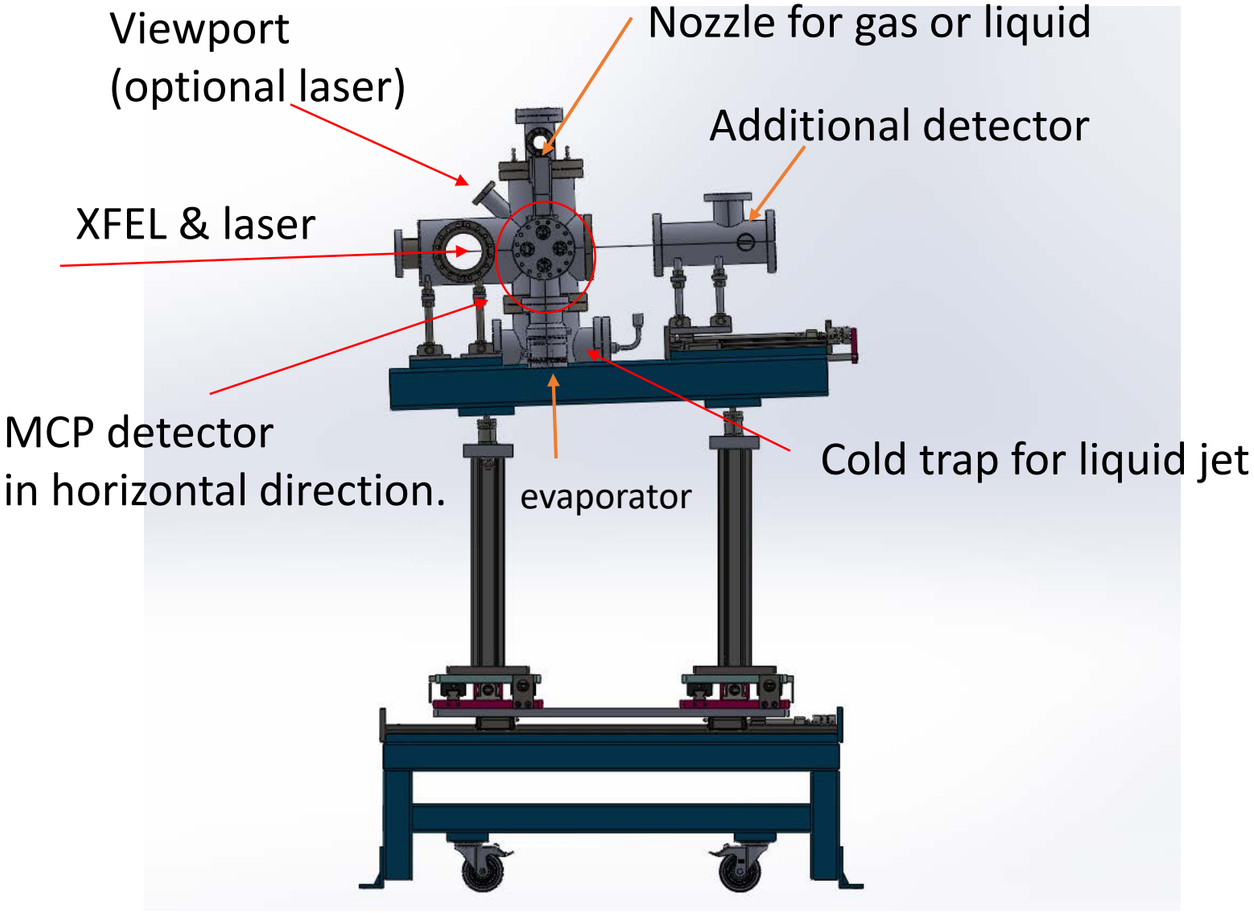
solid

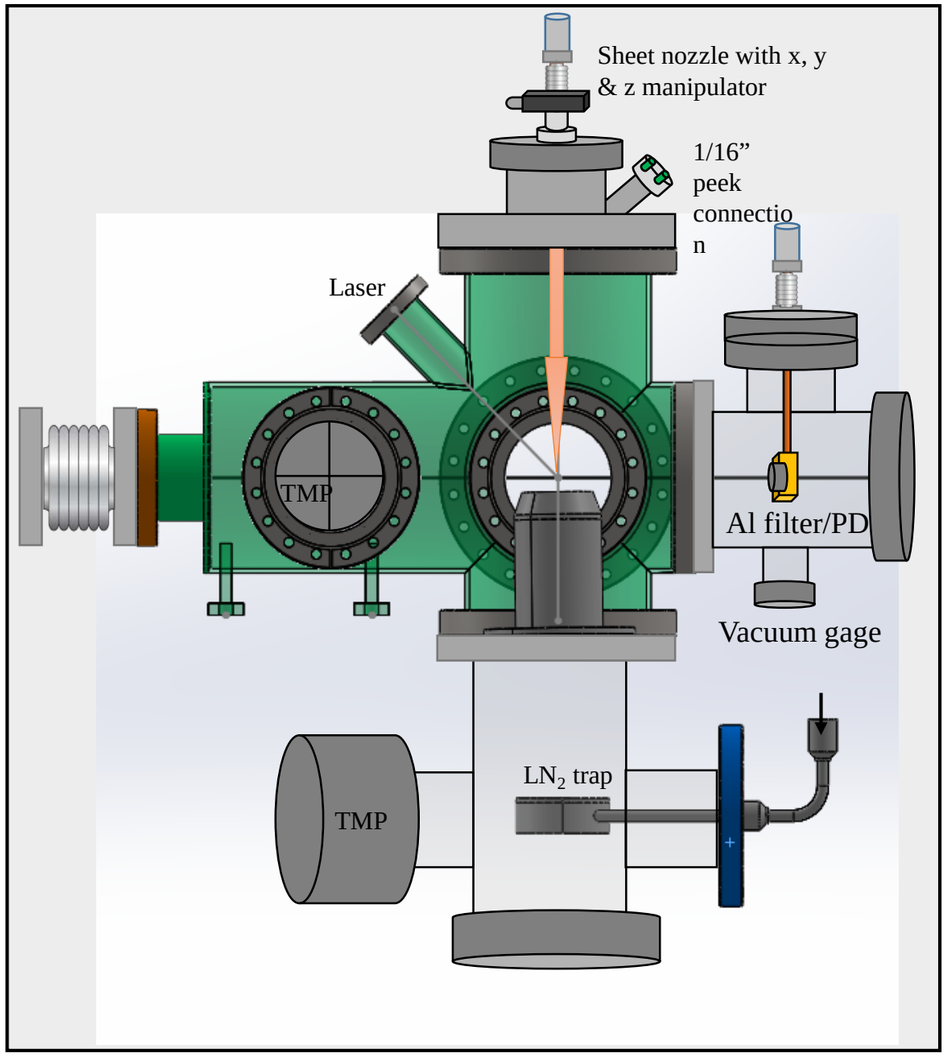
solution in water

Hole transferring to water delays E-H recombination.

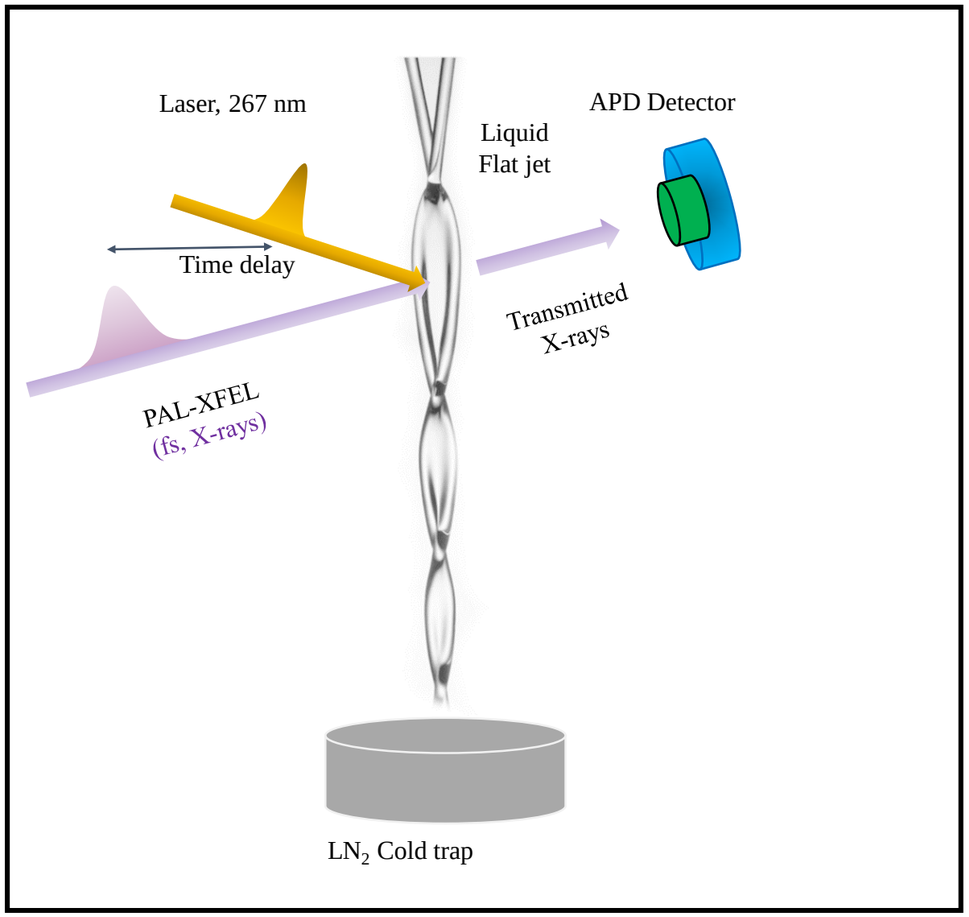


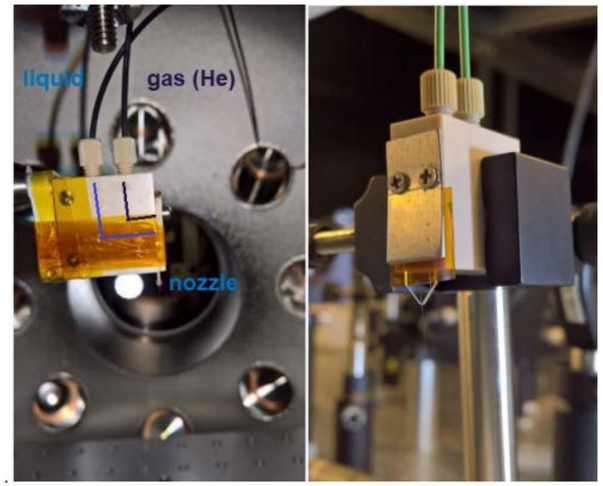
exchange setup for various condition

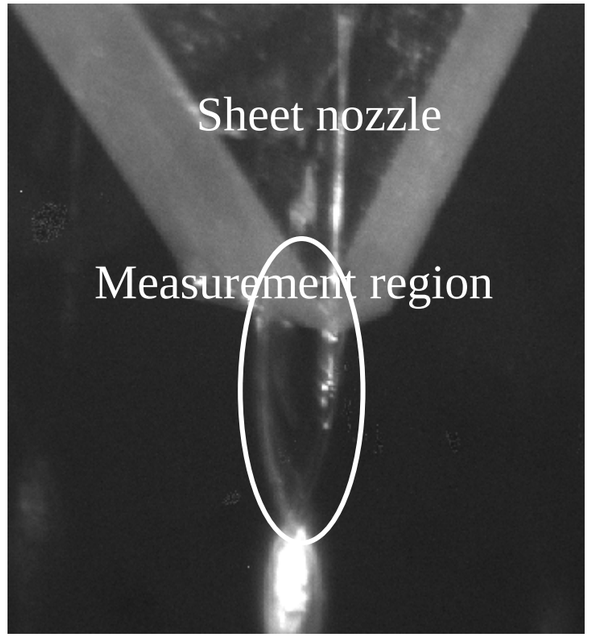




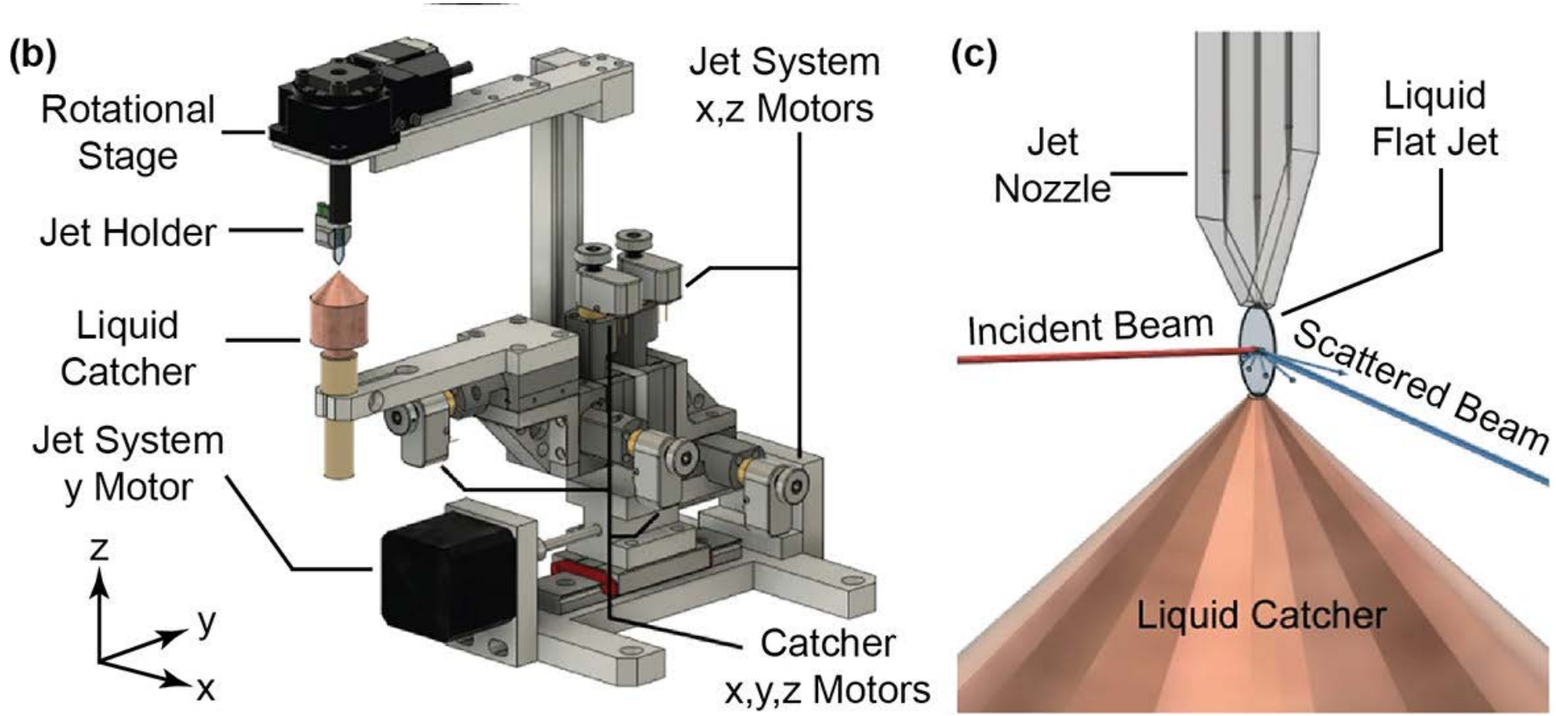
Liquid phase- flat jet





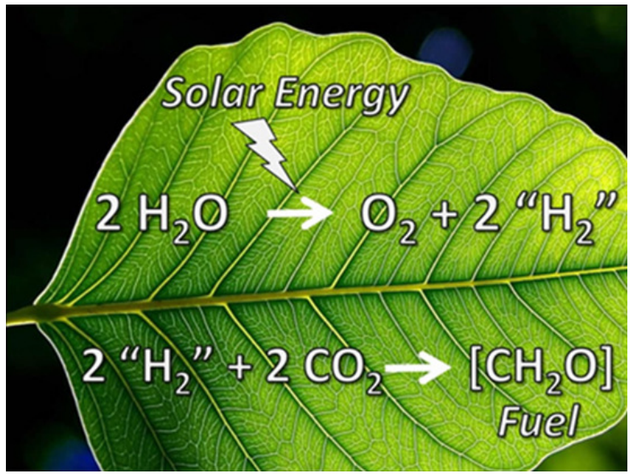


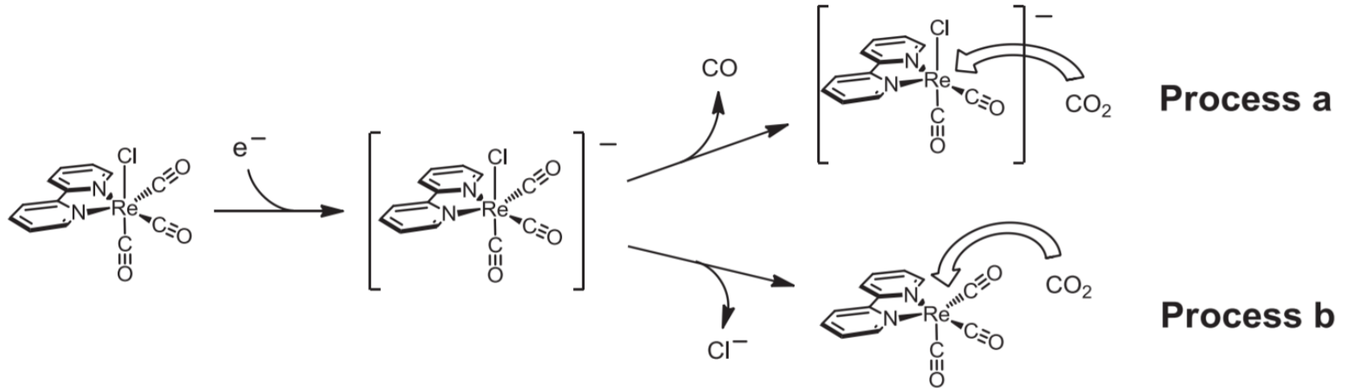
Liquid phase - Catcher upgrade

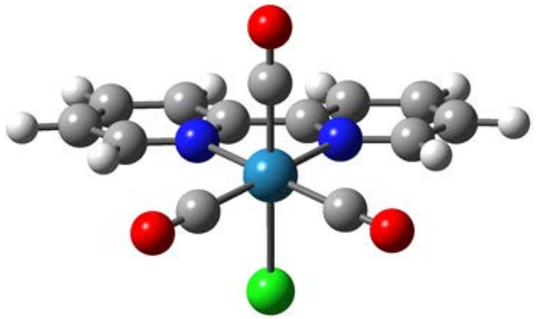


Rebpy(CO)$_3$Cl : the first step of photo-dissocation

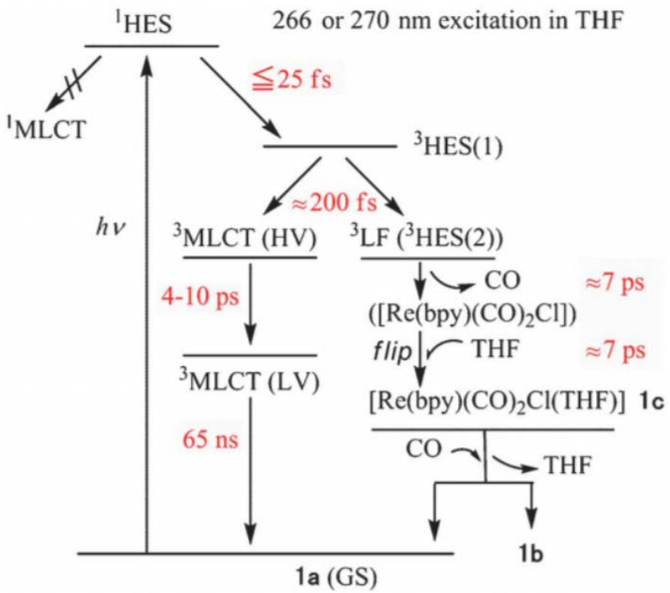
artificial photosynthesis







fac-Re[bpy][CO]$_3$Cl



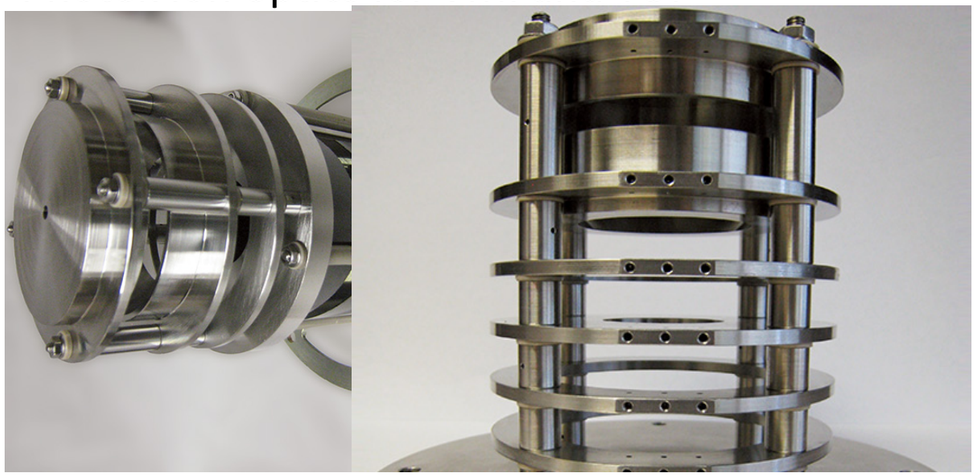
Rebpy(CO)$_3$Cl : Vapor phase experiment

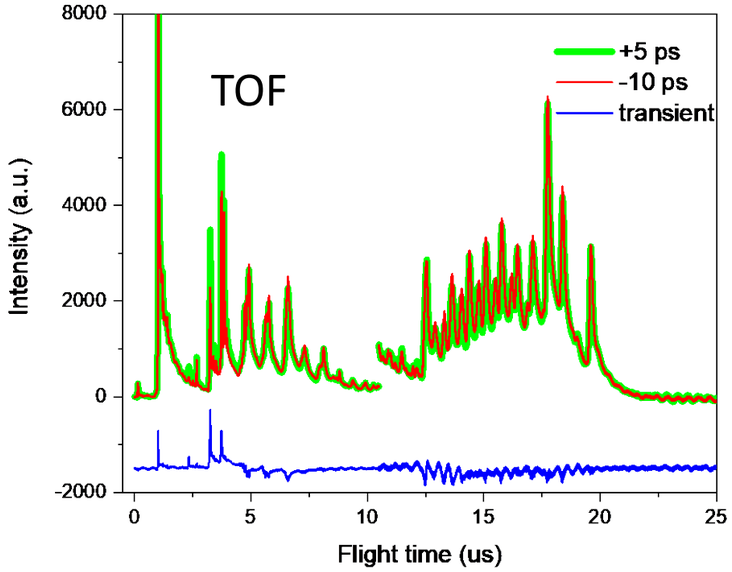
Sublimation using effusion cell
Up to 2000 deg.

10^{-7} ~ 10^{-5} Torr

organic molecule
stabilization time
sample consumption
cleaning

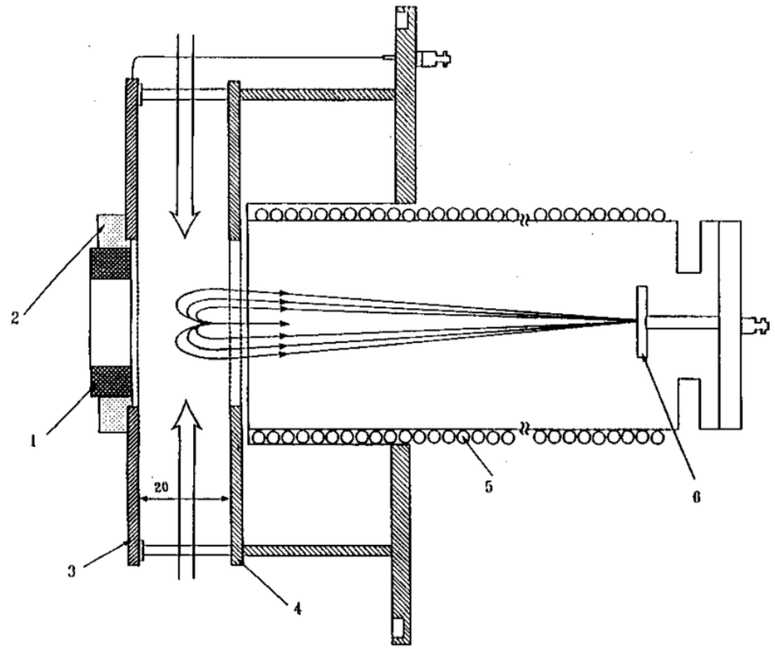
Photek Ion optics for VMI and TOF





Rebpy(CO)$_3$Cl : Vapor phase experiment

Magnetic bottle spectrometer



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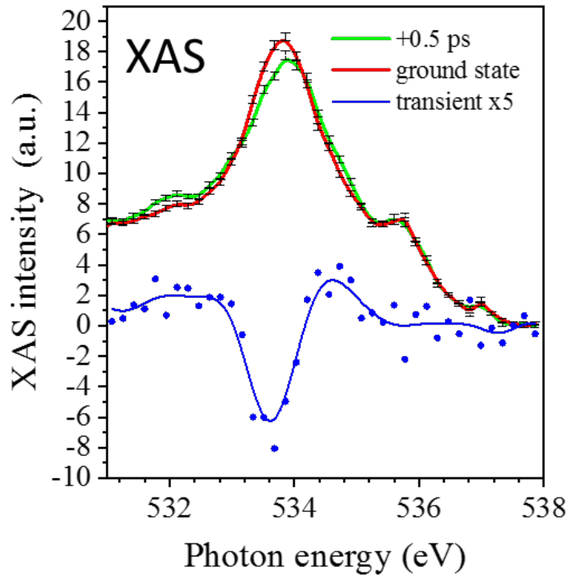
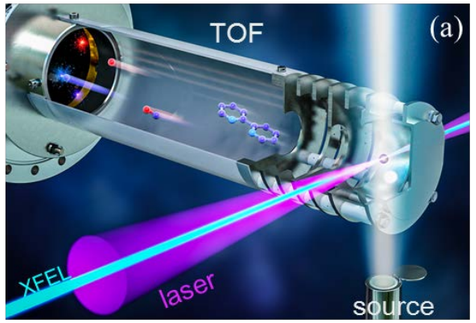
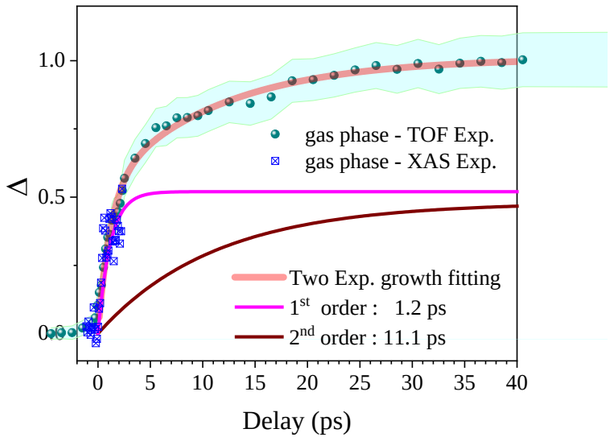


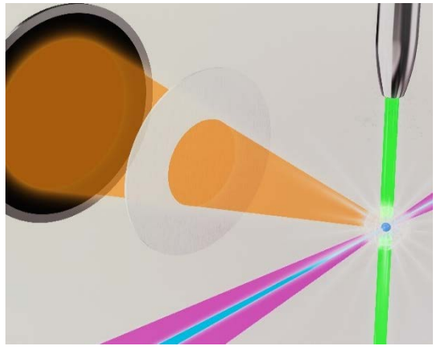
Rebpy(CO)$_3$Cl : cage effect in liquid

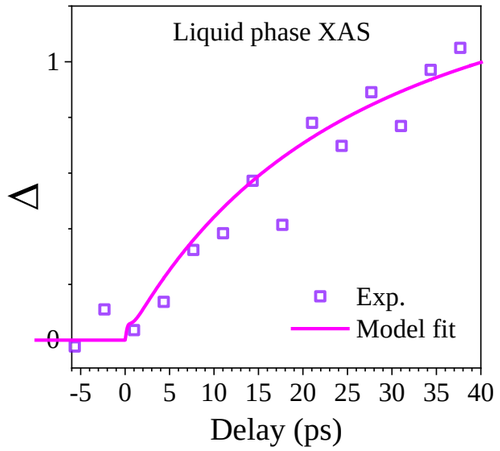
Vapor phase





Liquid phase





slow kinetics due to geminate recombination resulted from cage effect

Conclusion

- Many proposals related to energy materials are suggested, especially about catalytic reaction.
- We are expanding sample environment from solid to gas and liquid to create realistic reaction environment.
- Currently, we are focusing to setup stable liquid jet setup. And next step will be mixture of two reactant.