

# What I do...

Density functional theory

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

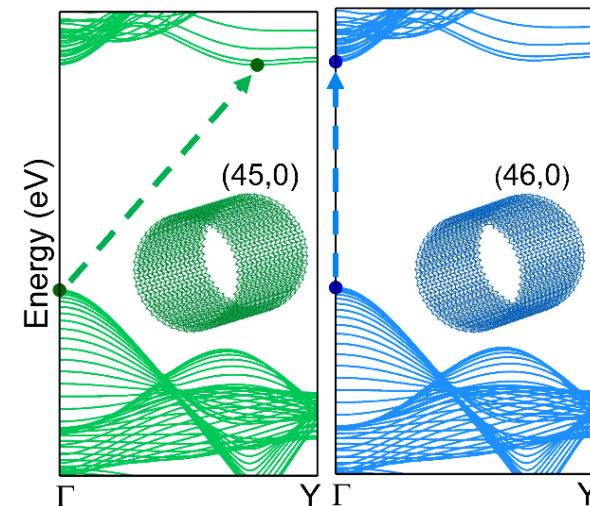
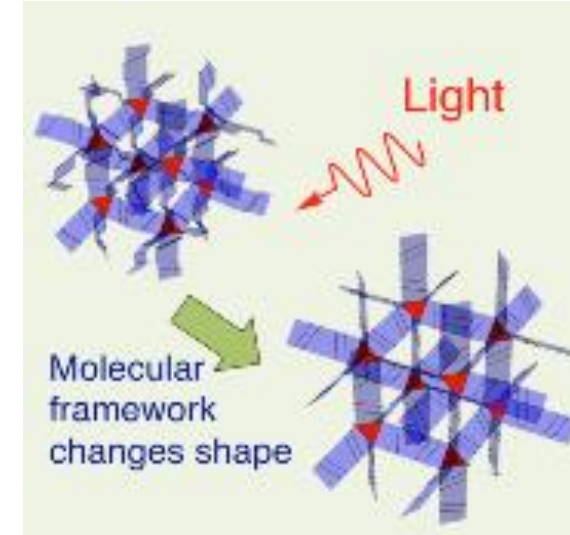
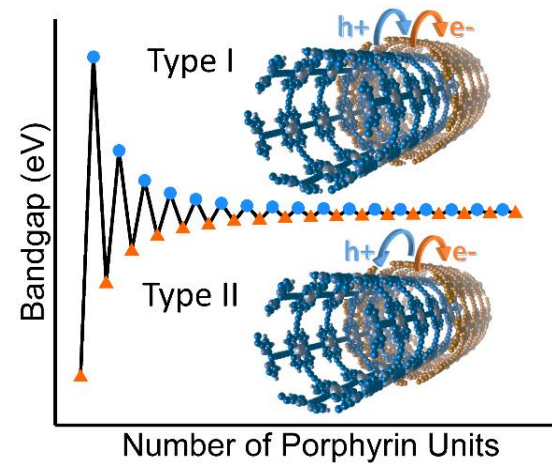
Computational materials science

Electron dynamics

$$i\hbar\frac{\partial}{\partial t}|\Psi(\mathbf{r},t)\rangle = \hat{H}|\Psi(\mathbf{r},t)\rangle$$

Molecular dynamics

$$\vec{F} = m\vec{a}$$



# What I want to do...

