

### Education

- 2012– **PhD Candidate in Chemistry program**, *The University of North Carolina – Chapel Hill*, Chapel Hill.
- 2008–2012 **Bachelor of Science with honor in Chemistry**, *University of Science and Technology of China*, Hefei, China.  
Specialized in Chemical Physics

### Professional Experience

- 2012– Graduate Research Assistant at University of North Carolina - Chapel Hill
- 2012–2013 Graduate Teaching Assistant at University of North Carolina - Chapel Hill
- 2011–2012 Undergraduate Research Assistant at University of Science and Technology of China

### Publications

Kyle G. Reeves, Yi Yao, and Yosuke Kanai. Diffusion quantum monte carlo study of martensitic phase transition energetics: The case of phosphorene. *The Journal of Chemical Physics*, 145(12), 2016.

Kyle G. Reeves, Yi Yao, and Yosuke Kanai. Electronic stopping power in liquid water for protons and  $\alpha$  particles from first principles. *Phys. Rev. B*, 94:041108, Jul 2016.

Yi Yao, Max L. Berkowitz, and Yosuke Kanai. Communication: Modeling of concentration dependent water diffusivity in ionic solutions: Role of intermolecular charge transfer. *The Journal of Chemical Physics*, 143(24), 2015.

Yi Yao and Yosuke Kanai. Reptation quantum monte carlo calculation of charge transfer: The nacl dimer. *Chemical Physics Letters*, 618:236 – 240, 2015.

Yi Yao, Yosuke Kanai, and Max L. Berkowitz. Role of charge transfer in water diffusivity in aqueous ionic solutions. *The Journal of Physical Chemistry Letters*, 5(15):2711–2716, 2014.