Prof. Jun Cheng
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Prof. Jun Cheng Jun Cheng received his PhD in Chemistry at the Queen's University Belfast, UK in 2008. , and the PhD project was simulating chemical reactions at solid-gas interfaces using density functional theory (DFT). He then moved to the University of Cambridge, first as a postdoc for two years developing a first principles method to calculate the free energies of electron/proton transfer reactions in aqueous solutions. In 2010-2013, he was awarded a prestigious junior research fellowship by Emmanuel College at Cambridge, which granted him freedom to pursue his interest in interfacial electrochemistry. He became a university lecturer at the University of Aberdeen, UK in 2013, and was soon rewarded the national "Thousand Youth Talents" Program Fund and took up a full professorship in Xiamen University, China. Over years, his research has shifted from computational surface science and heterogeneous catalysis, to method development in aqueous redox and acid-base chemistry, and to ab inito electrochemistry. His recent research work has been almost entirely devoted to developing electronic structure based methods for simulating chemical and physical processes at solid-liquid interfaces.

Jun Cheng has published 45 papers in peer reviewed journals and a book chapter, which has accumulated over 1300 citations. His H-index is 21. He has been invited to give talks at international conferences, including the Annual Meeting of the International Society of Electrochemistry, the American Chemical Society National Meetings.

Ab Initio Electrochemistry

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Electrochemistry is an old branch of science, and the renewed interest is largely due to its important relevance to the contemporary challenges on energy and environment. This offers a good opportunity for theoretical development of this interesting and challenging field. In this talk, I will present our recent work of development of a first principles method, combining density functional theory based molecular dynamics (DFTMD) and free energy perturbation theory, for computation of free energies of electron/proton transfer in aqueous solution, and the application to electrochemical interfaces.

References:

Jun Cheng*, et al. *Phys. Rev. Lett.* **2017**, *119*, 016801; *Phys. Rev. Lett.* **2016**, *116*, 086402; *Acc. Chem. Res.* **2014**, *47*, 3522; *Angew. Chem. Int. Ed.* **2014**, *53*, 12046; *Angew. Chem. Int. Ed.* **2014**, *126*, 1965.