AI^2 Electrochemistry

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Abstract: It is known that electrode materials undergo dynamic structural changes at *in-situ/in-operando* conditions. Yet, the majority of computational studies only consider the static structures of electrode materials. When the materials are submerged in liquid solution, dynamic solvation effects are often completely ignored, or treated with dielectric continuum models, often lacking validation. The situations are about to change. Thanks to the latest development of *in-situ* experimental techniques and state-of-the-art computational methods, dynamics of electrode materials has recently drawn more and more attentions in many research areas. In this talk, I will present our recent progress on modeling dynamic catalysis and electrochemistry using *ab initio* molecular dynamics (AIMD)[1-4]. In particular, when statistical sampling is getting too expensive, we develop efficient simulation protocols of **A**rtificial **I**ntelligence accelerated ***Ab Initio*** **M**olecular **D**ynamics (**AI^{2}MD**), enabled by the powerful Deep Potentials[5].

References:

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[5] H. Wang, L. Zhang, J. Han, W. E, *Computer Physics Communications* **2018**, *228*, 178.

Biography:

Prof. Jun Cheng did his PhD on computational surface catalysis at Queen's University Belfast, and then worked as a postdoc at the University of Cambridge on developing first principles methods for the computation of redox potentials and pKa's in aqueous solutions. In 2010, he received a junior research fellowship at Emmanuel College, Cambridge, and started his independent research in the field of ab intio electrochemistry. He became a university lecturer at the University of Aberdeen, UK in 2013, and was soon rewarded the National Start-up Program Fund and took up a full professorship in Xiamen University, China. In the past 10 years, he has developed novel *ab initio* methods for modelling electrochemical interfaces and has applied them to obtain fundamental understanding of interfacial processes at an atomistic level. He has published over 100 papers in peer-reviewed journals including Nat. Mater., Nat. Catal., Nat. Commun., Sci. Adv., PRL, etc., which accumulate around 4870 citations and his H-index is 39 according to Google Scholar.