



**SHENG BI**

*From France to Sweden*



Project: **Documentation on PinnWall- electrode models from integrating machine learning and atomistic simulation**

Research topic: **Chemistry**

Swedish Institution: **Uppsala University**

French Institution: **Phenix Lab in CNRS**

Dates of mobility: **06/02/2023 to 26/06/2023**

Program: **SFVE-A**



## PRESENTATION

Sheng Bi is a [Paris region fellowship](#) researcher at the [Phenix Lab](#) at [CNRS](#), in Paris. His research interests include developing molecular dynamics simulation algorithms for energy storage devices, discovering conductive MOFs for high-energy supercapacitors. His current research focuses on understanding the charge storage mechanisms of pseudocapacitive materials, particularly hydrous RuO<sub>2</sub> in aqueous electrolytes, using a multi-method computational approach. The project aims to provide molecular insights for the design of new energy storage systems. For more information, visit his [personal website](#).

## ACTIVITIES IN SWEDEN

Sheng Bi's main objective at the [TeC](#) group in the Uppsala University in Uppsala was to help integrate the [PiNN](#)-generated models into [MetalWalls](#), enabling the utilization of state-of-the-art electrode models in simulations. This tool serves as a bridge between MetalWalls and PiNN, two software packages developed by the team at Phenix Lab and the TeC group respectively. He was hosted by [Dr. Chao Zhang](#) and Chao's team that focuses on the physical chemistry of ionically conducting solutions and electrically charged interfaces for energy storage applications. During his mobility, he finalized the documentation of PiNNWall which was recently published in the article "[Heterogeneous electrode models from integrating machine learning and atomistic simulation](#)". He also had the opportunity to give a presentation entitled "Liquid-gated Transistors- Where and How (MD) Simulations and Experiments Meet" in a bi-weekly seminar held at the [Department of Chemistry](#) of the [Uppsala University](#) in front of around 50 students and researchers. He also attended the PhD mini-defense of [Lisanne Knijff](#) (a PhD student in TeC), and a research talk by [Prof. Saiful Islam](#) from the [University of Oxford](#).