

This presentation provides a quick review of the education, work, research background, and expertise of M. Aryanpour acquired in Iran and abroad. A summary of his PhD work " Ab-initio Modeling of Electrochemistry in PEM Fuel cells" will be presented first from a pure academic point of view. Then corresponding to the PhD work, the behind the scenes of the theoretical and computational challenges are discussed. The details include 1) how he developed a new computational method to accelerate locating the transition state of electron-transfer reactions using high-precision quantum calculations, 2) how he implemented the method to take advantage of High-Performance Computing (HPC). Following the PhD work, a sample of similar works and outputs are given in other research areas such as high-throughput screening of materials, and optimizing hybrid batteries for automotive industry. The presentation finishes with a list of computational technologies that he has been developing over years for multiple scientific subjects and applications.