



School of Nano Science (IPM)



Condensed Matter & Statistical
Physics Group (IPM)

Weekly Webinar

Quantum-mechanical characterization of interfacial processes on the cathode of Li-S batteries during discharge

Speaker: **Dr. Pouya Partovi-Azar**

Institute for Chemistry, Martin Luther University of Halle-Wittenberg, Halle, Germany

Increasing global energy demand brings about the need for more efficient energy-storage devices which are not only capable of storing significant amount of energy but also have low manufacturing costs. Lithium-based energy-storage devices have been serving our electric devices since 1970s. Now with the energy density of a typical Li-ion battery reaching a saturating value, new types of rechargeable batteries are highly ask for. Sulfur with its high theoretical lithium capacity of 1675 mAh/g is an abundant and low-cost element. Therefore, lithium-sulfur (Li-S) batteries are among the most promising candidates for next-generation energy-storage devices suitable for various applications, such as electrical vehicles. However, the available Li-S batteries suffer from low sulfur utilization and a poor cycle life which limit their applicability. From a chemical point of view, these problems are mainly related to the dissolution of Li-polysulfides, which form during lithiation of the sulfur cathodes (discharge), into the electrolyte. This leads to an irreversible capacity fade. Therefore, in the past years there has been a huge quest for finding suitable sulfur/carbon composite cathodes which not only mitigate the diffusion of Li-polysulfides away from the cathode but also ideally retain their original atomic structure after full charge/discharge cycles.

In this talk, I will present our recent quantum-mechanical investigations on characterisation of (polymeric) sulfur cathodes at fully charged stage as well as after initial lithiation reactions. Additionally, I will present our new line of research on the diffusion mechanism of Li cations in different electrolytes as well as through cathode-protecting layers. Throughout the talk, I will also introduce the 'machinery' we usually use in our theoretical investigations which enables us to directly compare our theoretical findings with experimental measurements through finite-temperature spectroscopy simulations.

Wednesday, 7 October 2020 (۱۳۹۹ مهر ۱۶), 14:00-15:00

Virtual Meeting Room (please log in as a guest):

<https://www.skyroom.online/ch/schoolofphysics/school-of-nano-science>

