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DIPARTIMENTO DI SCIENZE MATEMATICHE E INFORMATICHE, SCIENZE FISICHE E SCIENZE DELLA TERRA
Dottorato di Ricerca in Fisica

Appunti di Fisica '25

13 Marzo ore 15:00
Sala seminari, CNR-IPCF

Simulations of electrochemical systems with flexible electrode models

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Electrochemical energy storage devices, such as batteries and supercapacitors, play an important role in the ongoing energy transition. To further optimize their performance, a deep understanding of these devices is crucial. Atomistic simulations provide a unique opportunity to model these systems at the atomic scale under various operating conditions. Recent advancements have enabled explicit modeling of processes like supercapacitor charging.

However, current approaches often simplify electrode models, neglecting their mechanical dynamics, which may impact results, especially when coupled with ion dynamics. It is interesting to integrate Machine Learning Potentials, which are particularly effective for short-range interactions, with long-range physical models for describing electrostatic interactions.

Using recent advancements in the Performant Atomic Cluster Expansion model, the objective of this work is to understand the relationship between electrode dynamics, capacitance, and ion adsorption mechanisms. Our simulations showcased a notable decrease in charging time and increase in ions mobility for flexible electrodes models, motivating further exploration into the influence of electrode dynamics on supercapacitor performance. This research not only advances fundamental understanding but also holds promise for optimizing future energy storage device design and performance.

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