

セミナーのご案内

JSPS の短期招へい制度でパリ第6大学から来日予定の、M. Salanne 博士によるセミナー講演を企画しました。同博士は、イオン液体とカーボンナノチューブからなるスーパーキャパシターの分子動力学計算によって、キャパシターの増強効果の新たなメカニズムを提案するなど、その成果が大きな注目を集めています。

皆様どうぞお誘い合わせの上、奮ってご参加下さいますようご案内いたします。

日時：10月28日（月）16：30－17：30

会場：大学院・物質生産棟161演習室

共催：グリーンケミストリー連携教育研究センター

Title & speaker:

Understanding **the charging mechanism of supercapacitors** from molecular dynamics simulations

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Abstract:

A major challenge in moving towards sustainable and renewable energy sources is to develop lightweight and low-cost storage systems with the capability of leveling the cyclic nature of these sources to satisfy energy demands. Electrochemical double layer capacitors (supercapacitors) store energy at the electrolyte/electrode interface through reversible ion adsorption leading to higher charge/discharge rates and better cyclability but lower energy density compared to batteries. Nevertheless, the recent demonstration that ions from the electrolyte could enter sub-nanometer pores increasing greatly the capacitance opened the way for valuable improvements of the supercapacitors performances.

Despite the recent experimental and fundamental studies on that subject, the molecular mechanism at the origin of this capacitance enhancement is still not quite clear. We report here molecular dynamics simulations including two key features: the use of realistic electrode structures comparable with carbide-derived carbons and the polarization of the electrode atoms by the electrolyte. This original design of an electrochemical cell allows us to recover capacitance values in quantitative agreement with experiment and to gain knowledge about the local structure of the ionic liquid inside the pores (local ionic densities, local coordination numbers). Then, from the comparison between planar (graphite) and porous electrodes, we propose a new mechanism explaining the capacitance enhancement in nanoporous carbons.

References:

- Merlet, Rotenberg, Madden, Taberna, Simon, Gogotsi & Salanne, **Nature Materials**, 11, 306 (2012)
- Merlet, Pean, Rotenberg, Madden, Simon & Salanne, **J. Phys. Chem. Lett**, 4, 264 (2013)
- Limmer, Merlet, Salanne, Chandler, Madden, van Roij & Rotenberg, **Phys. Rev. Lett.**, 111, 106102 (2013)
- Merlet, Rotenberg, Madden & Salanne, **Phys. Chem. Chem. Phys.**, 15, 15781 (2013)