O 59: Invited talk (Mads Brandbyge)

Time: Thursday 9:30–10:15 Location: HE 101

Invited Talk O 59.1 Thu 9:30 HE 101

Electronic transport, Joule-heating, and current-driven dynamics in molecular contacts - theory and simulations — •Mads Brandbyge[1], Jing-Tao Lü[1], Tue Gunst[1], and Per Hedegård[2] — [1]Dept. of Micro and Nanotechnology (DTU-Nanotech), Technical Univ. of Denmark build. 345 east, DK-2800 Kongens Lyngby, Denmark — [2]Niels Bohr Inst., Univ. of Copenhagen, Universitetsparken 5, DK-2100, Denmark

Computer simulation and theoretical modelling play an vital role in the emerging field of nanoelectronics with device dimensions down to the molecular scale. Interpretation of experimental results and prediction of novel mechanisms for device operation poses many challenges especially for first principles theory, that is, calculations without fitting parameters. We have developed methods to address aspects of electron transport though nanoconductors from first principles based on density functional theory.

The influence of an electronic current on atomic dynamics is an important and intriguing problem in nanoelectronics. We have recently proposed an approach to molecular dynamics simulations which encompass Joule heating as well as current-induced forces not conserving the energy. We will discuss mechanisms where the current can lead to instabilities in the dynamics e.g. resulting in contact fluctuations or disruption at certain critial voltages. These mechanisms include "runaway" vibrational modes resulting from non-conservative forces, and a laser-type instability in certain types of molecular conductors (donor-acceptor-type systems).