

The 172nd MANA Special Seminar



Non-equilibrium theory of transport properties and energy conversion processes across nanostructured junctions Chair: Dr. Masakazu Aono (MANA Director-General)

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Single molecular bridge junctions and atomic wires form two distinct classes of nanostructured bridge junctions. A rough sketch of conduction mechanisms in these classes will be discussed first to give an idea of the most important material parameters of the problem. More details of the mechanism including inelastic scattering effects due to electron-phonon coupling and electronic correlation will be discussed next, which will be extended and combined with phonon thermal conductance calculation to give fully self-consistent theory of energy conversion processes and the local heating problem accompanying electric conduction across the junction. Possible highly efficient energy conversion using constriction structure of the junction will be discussed, shortly. While listed above are mostly theoretical, some examples of first principle calculation results will be presented, demonstrating its potential to simulate chemical reality.

Venue: Seminar Room #431, MANA Bldg.

Date: Oct 13th Wednesday Time: 15:30-16:15

Contact: International Center for Materials Nanoarchitectonics (MANA), Nakata (ex. 8806)

