Theoretical studies of the line shape of the inelastic tunneling spectroscopy

Tomomi Shimazaki and Yoshihiro Asai

National Institute of Advanced Industrial Science and Technology (AIST),
Umezono, 1-1-1, Tsukuba Central 2, Tsukuba, Ibaraki 305-8568, Japan
and
Core Research for Evolutional Science and Technology (CREST),
Japan Science and Technology Corporation (JST), Kawaguchi 332-0012, Japan

The single molecular conductance problem has been a matter of intense investigations among these years. Among all, inelastic current of molecule vibration origin has recently received much attention both experimentally and theoretically. There are some preceding calculations of the vibronic inelastic current [1,2], but finite bias voltage effects beyond the linear response scheme have not been discussed there. Serugeev et al. have addressed the importance of the problem [3]. We will discuss the finite bias effects on the vibronic elastic and inelastic currents. In order to take into account the bias effects, we adopt the nonequilibrium Green's function (NEGF) method and *ab initio* Hartree-Fock method [4]. The bias voltage effects are accompanied with the change of the molecular charge, which has the largest influence on the vibronic transport properties through single molecules.[5]
We will also derive important physical factors which control the line shape of the inelastic tunneling spectroscopy (IETS). [6]

[1] Y. Asai, Phys. Rev. Lett., 93, p246102, 2004; Phys. Rev. Lett., 94, p099901, 2005.
[2] T. Frederiksen, M. Brandbyge, N. Lorente, and A. Jauho, Phys. Rev. Lett., 94, p256601,2004.
[3] N. Sergueev, D. Roubtsov, and H. Guo, Phys. Rev. Lett., 95, p146803, 2005.
[4] T. Shimazaki, Y. Xue, M.A. Ratner, and K. Yamashita, J. Chem. Phys., 123,p114708, 2006.
[5] T. Shimazaki and Y. Asai, submitted to Phys. Rev. B.
[6] T. Shimazaki and Y. Asai, submitted to Phys. Rev. B.