Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Signal and thermal noise in [2]catenenane molecular electronic switches YONG-HOON KIM, Korea Institute for Advanced Study, SEUNG SOON JANG, YUN-HEE JANG, WILLIAM A. GODDARD III, California Institute of Technology — Due to the flexible nature of molecules, an important consideration in molecular electronics would be the influence of molecular vibrations on the device charge transport characteristics. Employing the first-principles matrix Green's function method combined with classical force-field molecular dynamics, we examine the effect of thermal vibrations on the switching in [2]catenane molecular electronic devices. Previously, we have identified frontier molecular orbitals that systematically shift within the two co-conforamations of bistable [2]catenane molecules, which results in the switching of the device when it is probed via a small bias. Here, we compute the charge transport characteristics of the molecule in the switch-on and switch-off configurations at different molecular dynamics snapshots, and find that the fluctuation of resonant transmission peaks in each conformation is smaller than the shift of the peaks between the two conformations. Thus, we confirm that the thermal noise does not mask the switching signal in the [2]catenane molecular electronic devices, which is in accordance with the experimental observation of the switching at the ambient condition.

Yong-Hoon Kim
Korea Institute for Advanced Study

Date submitted: 04 Dec 2004 Electronic form version 1.4