

RECTIFICATION
PROPERTIES OF A MOLECULAR
WIRE CAUSED BY ITS TERMINAL GROUPS

Ya.R. Zelinsky, E.G. Petrov

M.M. Bogolyubov Institute of Theoretical Physics,
Nat. Acad. Sci. of Ukraine
(14b, Metrolohichna Str., Kyiv 03143, Ukraine;
e-mail: yzelinsky@bitp.kiev.ua)

S u m m a r y

The current-voltage characteristics of a molecular wire are analyzed for a particular scheme of its energy levels. It is assumed that the levels of the lowest unoccupied molecular orbitals (LUMO) of internal wire units are energetically positioned much higher than the Fermi levels of metal electrodes and the LUMO levels of the terminal groups. The latter act as the specific intermediate donor and acceptor centers and control the current formation via the combined superexchange and sequential hopping mechanism of electron transfer. It is shown the blocking of the interelectrode current at a large voltage bias is caused by the strong electron-phonon interaction. Additionally, the rectification effect of a wire is obtained in the case of a nonvanishing donor-acceptor driving force, provided the superexchange mechanism dominates the current formation.