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Charge transfer along DNA molecule within Peyrard-Bishop-Holstein model NERANJAN EDIRISINGHE, Georgia State University, VADYM APALKOV, Georgia State University — Charge transport through DNA molecule is important in many areas ranging from DNA damage repair to molecular nanowires. It is now widely accepted that a phonon mediated hopping of a charge carrier plays a major role in charge transport through DNA. In the present study we investigate system dynamics within Peyrard-Bishop-Holstein model for the charge transfer between donor and acceptor sites. We found that an escape time of a charge, trapped at the donor state of the DNA strand, is very sensitive to the initial value of H-bond stretching. This suggests importance of ensemble averaging. Moreover sharp phase transitions were observed for escape time in parameter space of transfer integrals and phonon-charge coupling constant.

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