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Effect of molecular vibrations on charge transfer in polypeptide chains NIKOLAI SERGUEEV, ALEXANDER DEMKOV, University of Texas at Austin — We present first principles framework suitable for analyzing and understanding the effect of molecular vibrations on charge transfer in polypeptide chains. Our approach is based on density functional theory and Keldysh nonequilibrium Green's function formalism. This method allows us to treat both electrons and molecular vibrations (phonons) on equal footing in a self-consistent manner. The salient feature of our technique is that we consider the vibration of the whole polypeptide bridge. We present a numerical results for a charge transfer through alanine polypeptide chains of the various length and show that the electron tunneling is greatly affected when the interaction between electrons and molecular vibrations is taken into account. We also present a vibrational spectroscopy analysis and identify those vibrational modes of the alanine polypeptides involved into the inelastic charge transfer.

Nikolai Sergueev
University of Texas at Austin

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