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Effective Tunneling of Torsional Polarons in Short Molecules
EFTA YUDIARSAH, SERGIO ULLOA, Ohio University — We study the properties of polaron states in short molecules modeled by electron hopping among few sites and interacting *anharmonically* with rotational vibrational modes [1]. Our study includes numerical solution of the polaron models as well as analytical limiting expressions for different coupling regimes. We consider the interference of two types of hopping terms in the Hamiltonian, one that is angle dependent while the other one is not. Our model considers how dynamical coupling of torsional modes to orbital overlaps affects the transport properties of the electrons in molecules. We use different models of angle-dependent hopping with built-in asymmetries and find that they give opposite behavior in the polaron effective hopping constant: while polaron ground states are found to be typically more "massive" and have smaller effective hopping, asymmetries result in *larger* hopping with increasing restoring force of the vibrational modes. A more complex behavior is found for excited states. This behavior may have consequences for molecular transport experiments in flexible short molecules. Supported by NSF-NIRT.

[1] W. Zhang, A. O. Govorov and S. E. Ulloa, Phys. Rev. B 66, 060303(R) (2002)

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