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Nonadiabatic dynamics with quantum nuclei: Simulating charge transfer with ring polymer surface hopping

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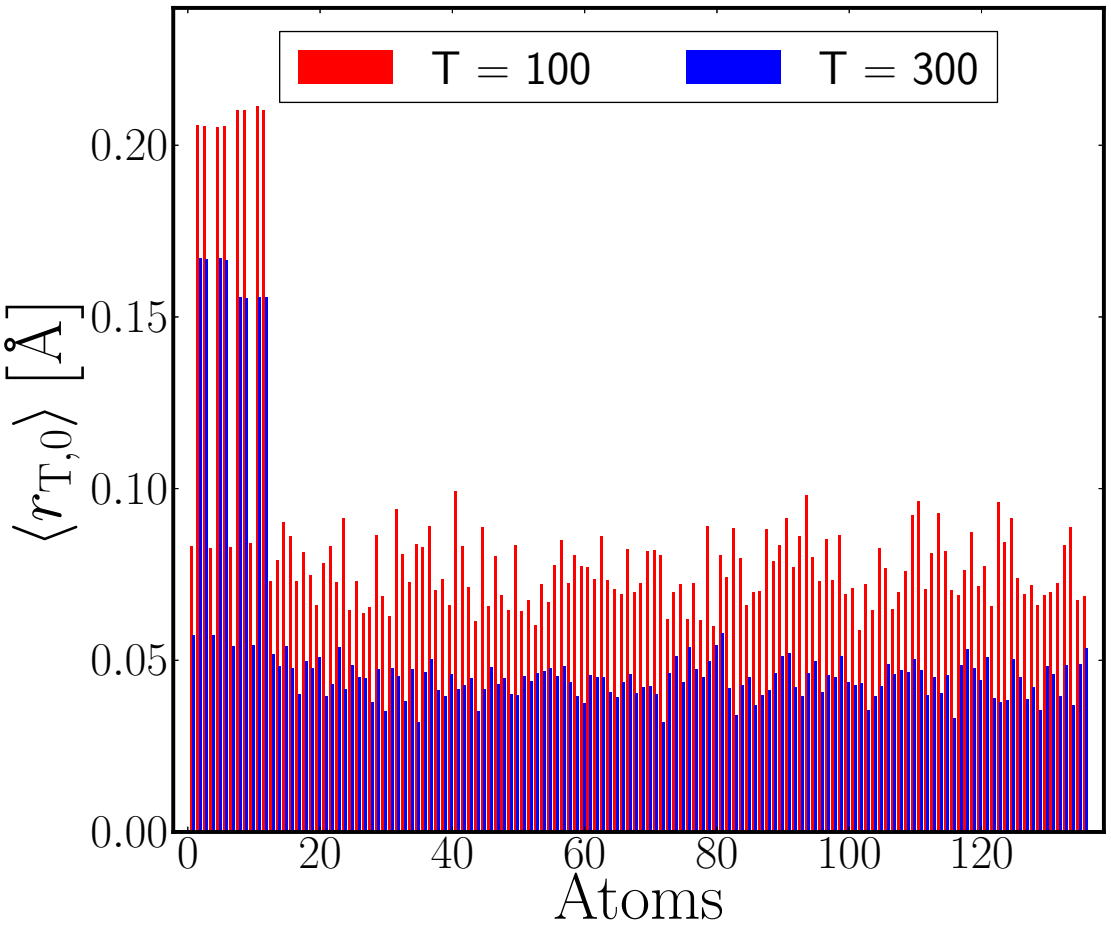

Fig. S1 The mean (trajectory and time averaged) radii of gyration of all the atoms in the supercell for hole transfer in ELM dimer at 100 K (red bars) and 300 K (blue bars) respectively. The first 12 atoms correspond to the ELM dimer (for ordering of the C and H atoms see the labels of xticks of Fig.(S2)) while the rest are Ne atoms representing a heat bath. As expected, the maximum increase occurs for the H atoms. The bar diagram clearly demonstrates the significance of nuclear tunneling, manifested by an increase in the radius of gyration, upon lowering the temperature from 300 K to 100 K.

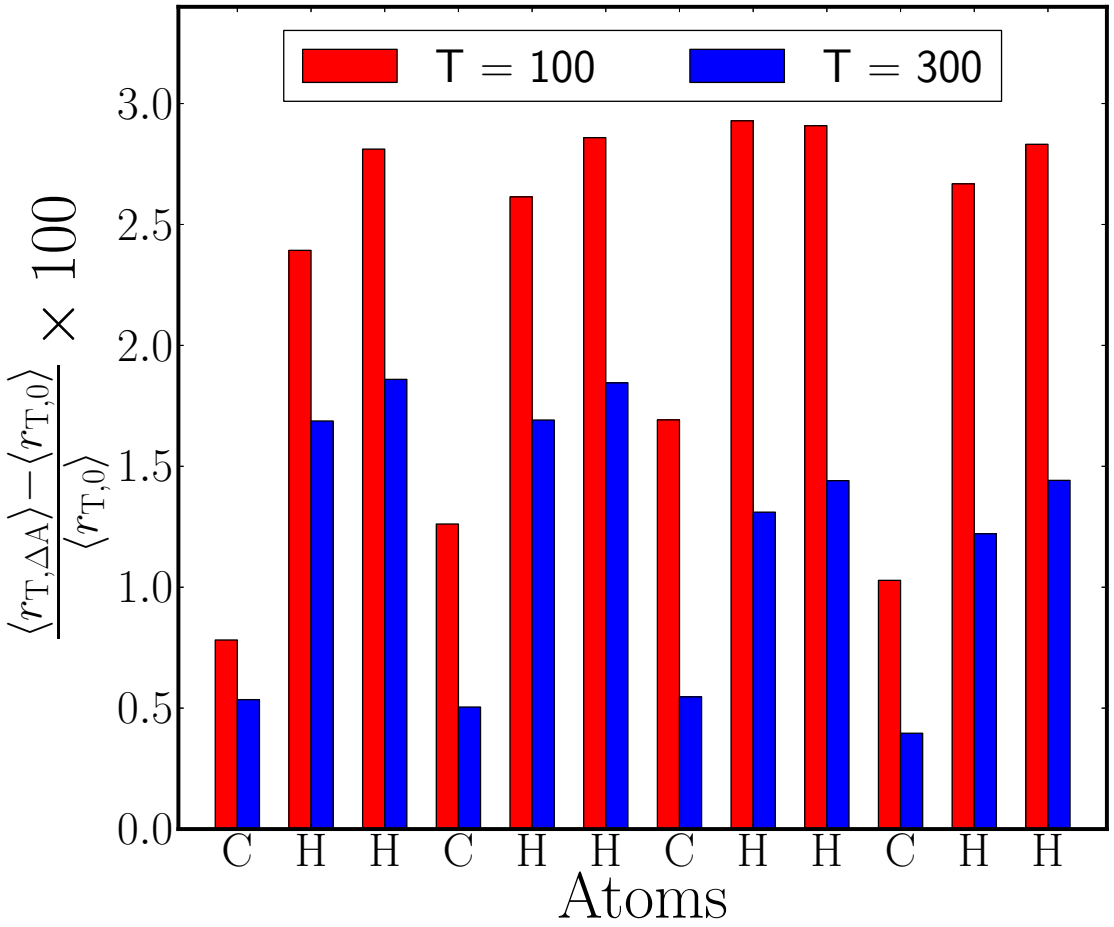

Fig. S2 The relative increase in radius of gyration of the atoms of the ELM dimer at 300 K and 100 K upon increasing the driving force ($-\Delta$A) from 0 to 400 meV and 300 meV respectively. The relative increase is much larger at 100 K compared to 300 K signifying the importance of nuclear tunneling at lower temperatures.