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Soliton migration along *trans*-polyacetylene backbone[1] MINGHAI LI, YONGWOO SHIN, XI LIN, Boston University — We compute the minimum energy paths and activation barriers for the soliton migration process along trans-polyacetylene backbone via the Su-Schrieffer-Heeger (SSH) model and *ab initio* calculations. Our results confirm the conventional consensus that soliton hops over two CH sites in one single step, maintaining wavefunction nodal structures at intermediate CH sites. Standard SSH parameters give rise to negligible migration barriers, which increases exponentially as the localization width decreases. Favoring the opposite elastic strain as the boundaries, soliton prefers staying at the center of an open chain; this ground state energy increases linearly when the chain length decreases. Starting at the center and moving towards the chain termination, soliton first sees a quadratic wash-board energy landscape when it is far away from the boundary and then smoothly switches to an exponentially increased wash-board energy landscape when it is in the vicinity of the boundary due to its localization width shrinkage. The local minima energy has a larger exponent compared to that of the activation barrier so they cross each other at a certain point, beyond which the barrier disappears and solitons cannot get closer to the boundary.

[1]Honda R&D

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