Supplementary Material

Vibrational Characteristics of DNA Nanostructures Obtained Through a Mass-weighted Chemical Elastic Network Model

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Symmetry-constrained elastic network model (SCENM)

How to construct the reduced connectivity matrix in SCENM. In this paper, in case of DNA buckyball structure, because of its icosahedral symmetric property, SCENM was additionally applied in order to effectively analyze intrinsic modes of buckyball structure by using only a three-point-star (3PS) tile with connectivity information of neighboring tiles instead of handling the whole buckyball structure. As shown in Figure S1, symmetric boundary condition including intraconnectivity from a single 3PS tile and interconnectivity from three neighboring tiles can be applied to construct the reduced connectivity matrix $K_{reduced}$ for a single 3PS tile such that

$$K_{reduced} = K_{1,1} + K_{1,2}R_2 + K_{1,3}R_3 + K_{1,4}R_4$$

Based on this methodology, the computational cost of normal mode analysis can be reduced by the factor of 60.

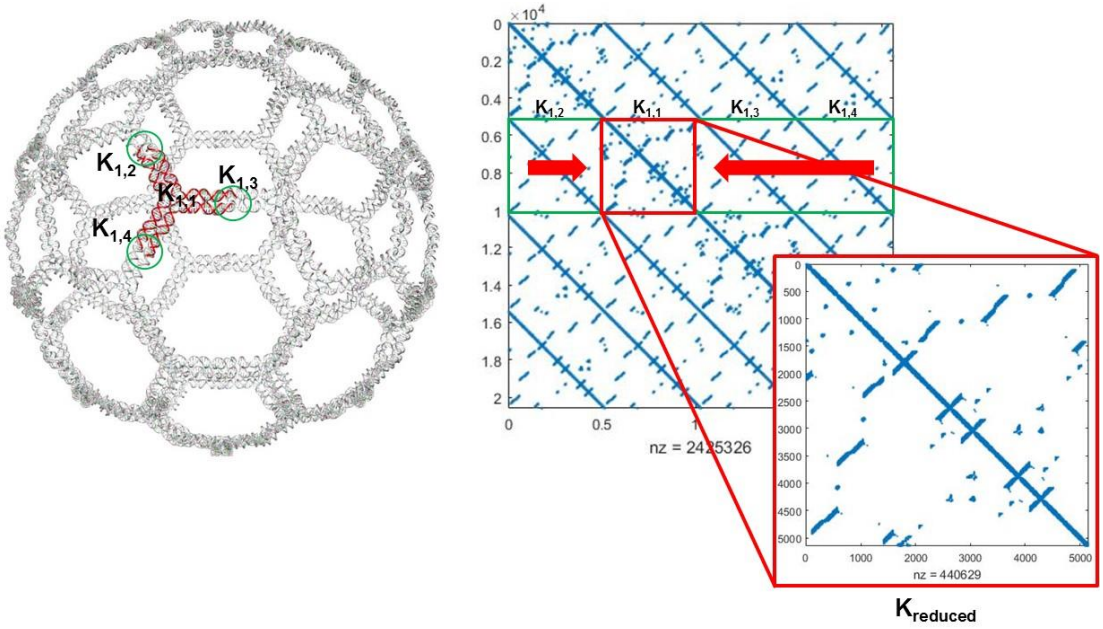

Figure S1. Connectivity information of the buckyball structure