

To study the knotting complexity of a structure, we introduce a novel dynamic relaxation model to simplify the knot structure without changing its knotting complexity. In this model, both the 3' and 5' ends of a 3D ssOrigami model are fixed while the remaining part of the strand falls under simulated gravity. The falling process will relax the unknotted crossings, and thus simplify the diagram. For example, if a structurally "complex" 3D knot model is actually an unknot (crossing number 0), the relaxation will simplify the model into an untied loop (unfolding). On the other hand, if a 3D knot model is knotted, the crossings will be kept during the falling process.

[Movie-1] Dynamic animation to demonstrate the knot relaxation process of a simple DNA hairpin.

[Movie-2] Dynamic animation to demonstrate the knot relaxation process of a paired double helical DNA with antiparallel crossovers analogue.

[Movie-3] Dynamic animation to demonstrate the knot relaxation process of RNase (PDB: 1GQV).

[Movie-4] Dynamic relaxation to demonstrate the knot relaxation process of Telomerase (PDB: 3KYL).

[Movie-5] Dynamic relaxation to demonstrate the knot relaxation process of Group II Intron (PDB: 3EOH).

[Movie-6] Dynamic relaxation to demonstrate the knot relaxation process of 16S rRNA (PDB: 1L94).

[Movie-7] Dynamic relaxation to demonstrate the knot relaxation process of acetohydroxy acid isomeroreductase (PDB: 1YVE-L).

[Movie-8] Dynamic relaxation to demonstrate the knot relaxation process of an anti-parallel ssOrigami model shown in Fig. S4-8.

[Movie-9] Dynamic relaxation to demonstrate the knot relaxation process of a parallel ssOrigami model with 16bp crossover distance shown in Fig. S5-2.

[Movie-10] Dynamic relaxation to demonstrate the knot relaxation process of the 3×3 ssOrigami model.

[Movie-11] Dynamic relaxation to demonstrate the knot relaxation process of the 4×4 ssOrigami model.

[Movie-12] Dynamic relaxation to demonstrate the knot relaxation process of the 5×5 ssOrigami model.

[Movie-13] Dynamic relaxation to demonstrate the knot relaxation process of the strip-shape ssOrigami model.

[Movie-14] Dynamic relaxation to demonstrate the knot relaxation process of the rectangle-shape ssOrigami model.

[Movie-15] Dynamic relaxation to demonstrate the knot relaxation process of the triangle-shape ssOrigami model.

[Movie-16] Dynamic relaxation to demonstrate the knot relaxation process of the rhomboid-shape ssOrigami model.