

## Coarse-grained modelling of DNA and DNA self-assembly

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Deskripsi Lengkap: <https://lib.ui.ac.id/detail?id=20425067&lokasi=lokal>

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### Abstrak

This thesis presents a novel coarse-grained model of DNA, in which bases are represented as rigid nucleotides. The model is shown to quantitatively reproduce many phenomena, including elastic properties of the double-stranded state, hairpin formation in single strands and hybridization of pairs of strands to form duplexes, the first time such a wide range of properties has been captured by a coarse-grained model. The scope and potential of the model is demonstrated by simulating DNA tweezers, an iconic nanodevice, and a two-footed DNA walker. The first time that coarse-grained modelling has been applied to dynamic DNA nanotechnology.