

FREIE UNIVERSITÄT BERLIN
Fachbereich Mathematik und Informatik

Promotionsbüro, Arnimallee 14, 14195 Berlin

DISPUTATION

Mittwoch, 14. Dezember 2016, 14.30 Uhr

**Ort: Zuse-Institut Berlin (ZIB)
Seminarraum (R2005, Erdgeschoss)
Takustr. 7, 14195 Berlin**

Disputation über die Doktorarbeit von

Herrn Vedat Durmaz

**Thema der Dissertation:
Atomistic Binding Free Energy Estimations
for Biological Host-Guest Systems**

**Thema der Disputation:
A critical assessment on Gaussian coarse-grained DNA models**

Die Arbeit wurde unter der Betreuung von **PD Dr. M. Weber** durchgeführt.

Abstract: In the fields of structural biology and material science, DNA models represent a well-established approach to the depiction and prediction of the three-dimensional structure of DNA molecules ensuing from their nucleic acid base sequence. Insofar, these models are convenient for both the understanding of biological processes including gene regulation by transcription factors as well as for the development of suitable drugs, DNA nanocarriers, and nanostructures. Among a highly diverse set of available DNA models, those coarse-grained on the base level turn out to be particularly balanced regarding the trade-off of model accuracy versus computational effort. The talk will start with some basic ideas of coarse-grained DNA models and afterwards focus on the physical, sequence-dependent cgDNA model developed by John Henry Maddocks and co-workers. For oligomers from tens up to few hundred bases this model is claimed to provide a quick estimate of its ground state along with a convenient Gaussian equilibrium probability density function. Conclusively, the validity of assumptions related to Gaussianity and structural symmetry relations will be elaborated using spectral clustering methods.

Die Disputation besteht aus dem o. g. Vortrag, danach der Vorstellung der Dissertation einschließlich jeweils anschließenden Aussprachen.

Interessierte werden hiermit herzlich eingeladen

Der Vorsitzende der Promotionskommission
PD Dr. M. Weber