Statistical study of linear heteropolymers

1996 Fiscal Year Final Research Report Summary

Statistical study of linear heteropolymers

Research Project

Project/Area Number

07640508

Research Category

Grant-in-Aid for Scientific Research (C)

Allocation Type

Single-year Grants

Section

一般

Research Field

物性一般(含基礎論)

Research Institution

Kanazawa University

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diblock polyampholyte / protein folding / Monte-Carlo simulation / pairing transition

Research Abstract

The understanding of the conformational transitionas of biopolymers is a fundamental problem of statistical physics. Protein as well as nucleic acid folding are the main puzzling problems of biological importance. In order to tackle such problems, we undertook a systematic study of polyampholytes so as to understand the relation between the sequence of charges and the observed conformations. The term polyampholyte (designed as PA hereafter) is a generic name describing a polymer chain bearing positively and negatively charged monomers in a given sequence. A coil-globule transition was observed in an alternate polyampholyte. It was recognized that alternate sequences were highly specific and that random sequences should not exhibit any coil-globule transition. For globally neutral sequences, which is the relevant situation to proteins, our general aim is to understand what, in a given sequence, is relevant to conformational transitions. Note that nucleic acids are no PA but polyelectrol ytes (any nucleotide bears the same negative charge), so that the electrostatic interactions do not depend on the sequence of bases but merely on the ionic force.
Diblocks and alternate sequences are the two extreme cases among random sequences. For an alternate PA, it is just 0 (except of course for the two monomers in the middle of the chain, but their contribution becomes negligible as the chain length grows). Although long diblocks are far from being the rule among biopolymers (and hereafter it will clearly appear why they don't exist in nature at ordinary temperature) they are nonetheless relevant to the physiccs of biopolymers for the following reason : any sequence of charges generally contains small diblocks spread throughout the chain. The longer the chain, the longer the diblocks. These small diblocks should undergo the earliest transitions (i. e. at the highest temperatures). It seems therefore important to understand the nature of the transitions occurring in diblocks as a function of their size. This is the main issue of the present work.▲ Less

Research Products (50 results)

All Other

All Publications (50 results)

[Publications] K.Uehara: "Frist-principle molecular dynamics calculation of selenium clusters" J. Mol. Simulation. 18. 385-394 (1997)

[Publications] K.Uehara: "First-principles molecular dynamics simulations for Se_8 and Se_8^+ clusters" J. Mol. Simulation, in press.

[Publications] S.Makino: "Classical Molecular Dynamics for the Formation Process of a Fullerene Molecule" J. Phys. Chem. Solids, in press.

[Publications] T. Hashimoto: "Structural Transformations of Ice at High Pressures via Molecular Dynamics Simulations" J. Mol. Simulation. 18. 115-132 (1996)

[Publications] T.Hashimoto: "Structural transformations of ice at normal and high pressures via molecular dynamicssimulations" Proc. PCI'96, in press.

[Publications] T.Hashimoto: "Structural transformation of oce at high pressures via molecular dynamics simulation II" J. Mol. Simulation. 18. 395-406 (1997)

[Publications] J.Habasaki: "Fracton Exciattion and Levy Flight Dynamics in Alkali Silicate Glasses" Phys. Rev. B, in press.

[Publications] J. Habasaki: "Relaxation processes and the mixed alkali effect in alkali metasilicate glasses" Proc. MRS Fall Meetings, in press.

[Publications] J. Habasaki: "MD study of the mixed alkali effect in terms of the potential surfase in the lithium-potassjum metasilicate glass" J. Non-Cryst, Solids, in press.

[Publications] J. Habasaki: "Mixed Alkali Effect in Alkali Metadilicate Glasses" Proceedings of YKIS96, in press.

[Publications] 巾崎潤子: "アルカリケイ酸塩ガラスの構造とダイナミックス-ガラス転移,緩和現象と混合アルカリ効果-" 高分子論文集. 53. 774-787 (1996)

[Publications] T. Muranaka: "Study on the β peak of χ" for a two-dimensional supercooled fluid state via molecular dynamics simulation" J. Mol. Simulation. 16. 387-397 (1996)

[Publications] T.Muranaka: "Coupling between Jump Motions and Correlated Motions" Proceedings of YKIS96,. (in press).

[Publications] 橋本保: "氷に関する最近の分子動力学シミュレーション-氷の構造相転移-" 日本雪氷学会誌 雪氷. 58. 422-424 (1996)

[Publications] Y. Hiwatari: "Molecualr-dynamics simulation for the formation process of a fullerene molecule" RIKEN Rev. 14. 7-8 (1996)

[Publications] K. Uehara: "First-principle molecular dynamics calculation of selenium clusters" Proceedings of the ISSPIC 8. (in press).

[Publications] T. Odagaki: "Glass transition singularities and slow relaxation" Mat. Res. Soc. Symp. Proc.367. 337-346 (1995)

[Publications] Y. Hiwatari: "Slow Dynamics in Supercooled Fluids" J. Mol. Liquids. 65/66. 123-130 (1995)

[Publications] Y.Hiwatari: "Molecular-Dynamics Study of Supercooled Liquids and the Theory of the Glass Transition" J. Phys. Soc. Jpn., Comp. Physics as a New Frontier in Condensed Matter Res.329-339 (1995)

[Publications] J. Habasaki: "MD study of the mixed alkali effect in a lithium-potassium metasilicate glass" J. Non-Crystalline Solids. 183. 12-21 (1995)

[Publications] T. Muranaka: "β relaxation in a highly supercooled state via molecular dynamics simulation" Phys. Rev.E51. R2735-R2738 (1995)

[Publications] J. Habasaki: "Origins of the two-step relaxation and the boson peak in an alkali silicate glass studied by molecular-dynamics simulation" Phys Rev.E52. 2681-2687 (1995)

[Publications] J. B. Imbert: "Conformational Transitions of a Diblock Polyampholyte in 2 and 3 Dimensions" submitted to Europhysucs Letters.

[Publications] N. Urakami: "Multicanonical Monte Carlo Simulation of a Polymer with Stickers" J. Phys. Sci. of Japan. 65. 2694-2699 (1996)

[Publications] N. Urakami: "The distribution of the Gyration Radius of a Model of Ionomer Studied by Multicanonical Monte Carlo Simulation" Mol. Simylation,. (in press).

[Publications] N.Urakami: "Monte-Carlo simulation of a polymer with stickers・・・Initial relaxation and free energy calculations・・・" Proceedings of YKIS96,. in press.

[Publications] K.Uehara: "First-principle molecular dynamics calculation of selenium clusters" J.Mol. Simulation. 18. 385-394 (1997)

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