АКАДЕМИЯ НАУК РЕСПУБЛИКИ УЗБЕКИСТАН
ИНСТИТУТ ХИМИИ И ФИЗИКИ ПОЛИМЕРОВ
ПРОБЛЕМНЫЙ СОВЕТ “ВЫСОКОМОЛЕКУЛЯРНЫЕ СОЕДИНЕНИЯ”
ОБЩЕСТВО ХИТИНОЛОГОВ УЗБЕКИСТАНА

Международная конференция

«ФУНДАМЕНТАЛЬНЫЕ И ПРИКЛАДНЫЕ АСПЕКТЫ ИССЛЕДОВАНИЙ ХИТИНА И ЕГО ПРОИЗВОДНЫХ»

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ON OBTAINING BINARY POLYELECTROLYTE COMPLEXES OF CHITOSAN BOMBYX MORI WITH POLYANION

[2]Khudoyberdiyev Sh. Sh., [1]Vokhidova N. R., [1]Nurgaliyev I.N., [1]Rashidova S. Sh.
[1]Institute of Chemistry and Physics of Polymers of Scientific Academy of Uzbekistan
[2]Bukhara State University

In recent years, there has been an increase in demand for new materials based on polyelectrolyte complexes (PEC), the focus of scientists is attracted by the capability of chitosan (CS) complexes with specific properties with other polyanions. PEC represent a special class of polymeric substances formed as a result of cooperative reversible reactions of the combination of oppositely charged ions [1-2].

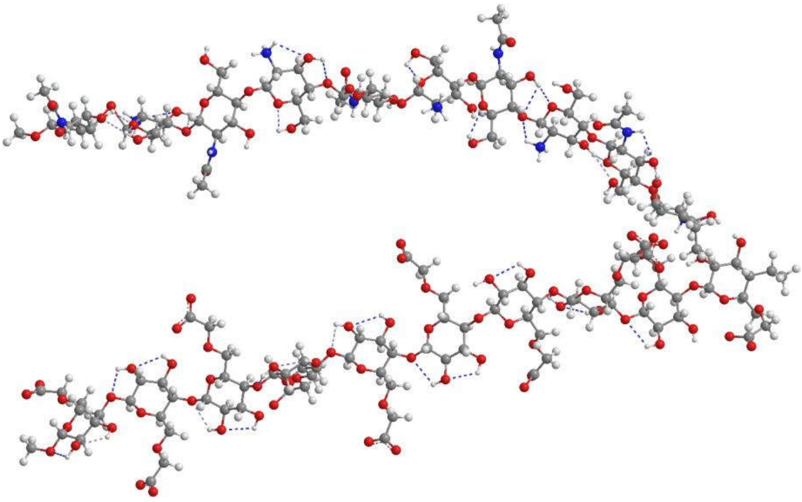
Upon receipt of chitosan PEC, the complexes tend to aggregate due to charge neutralization, therefore, in order to avoid aggregation and control the size of nanoparticles, at least two conditions are mandatory: polyelectrolyte solutions must be diluted, and one of the polyions must be in excess so that the following inequality is preserved:$(n+/n-) \neq 1$ [3].

The interaction of macromolecules of CS polycationite with the Na-CMC polyanion was studied by the conductometric method. Then, the electrical conductivity of stoichiometric and non-stoichiometric PEC, obtained by changing the molar ratios of CS and Na-CMC in the range of 1:0.1÷1:0.5, was investigated. It should be noted that a decrease in electrical conductivity was observed on the titration curve in the ratio CS/Na-CMC=1:0.34 mol, indicating a stoichiometric interaction, where positively charged protonated amino groups (NH_3^+) of CS macromolecules are completely compensated by carboxyl groups ($-COO^-$) of Na -CMC.

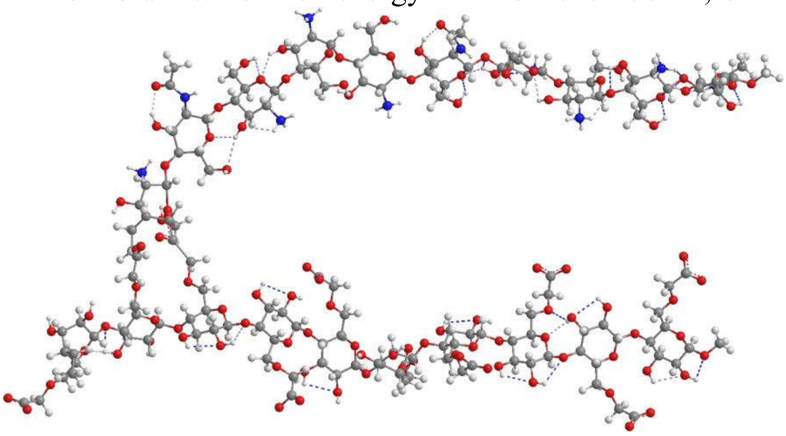
Theoretical calculations of the formation of interpolyelectrolyte complexes

Theoretical calculations also make it possible to calculate possible interactions between compounds, the possibility of forming various kinds of bonds, complexes, agglomerates, cluster and nanostructures. In the present study, we investigated the charge distribution of amino groups in chitosan chains of various lengths depending on the degree of deacetylation, the reactivity of the acetamide and amino groups in the composition of chitosan, the interaction of chitosan with Na-CMC, and the stability of their interpolymer complexes.

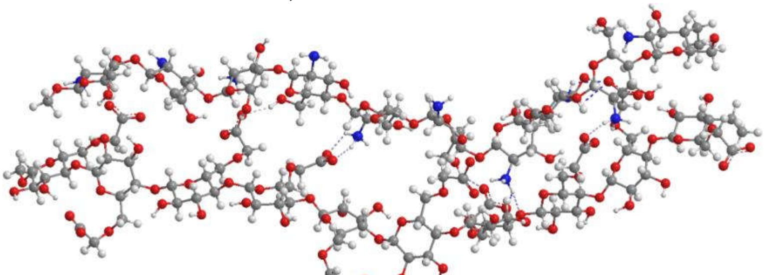
The main interaction between CMC and chitosan changed from a weak Van-der-Waals interaction to a strong electrostatic interaction linking the chains of the two polymers into a compact structure (Figure 1).



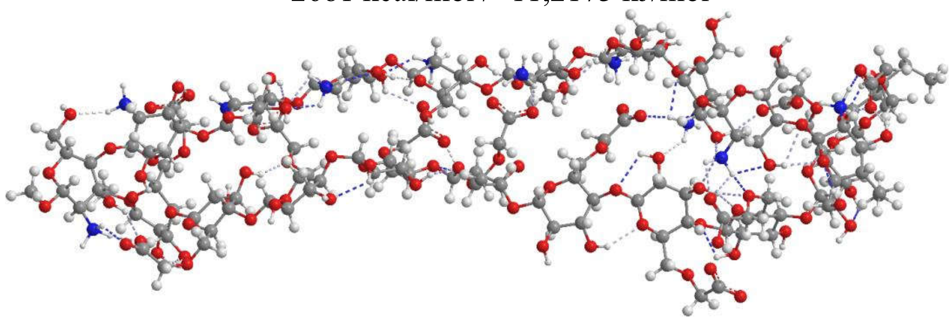
Interaction of a chain of 10 chitosan units containing 5 acetamide groups with a chain of 10 Na-CMC units. Iteration energy = -3249 kcal/mol/-13,59382 kJ/mol



Interaction of a chain of 10 units of chitosan containing 3 acetamide groups with the chain and 3 10 units of Na-CMC. Iteration energy = -3474 kcal/mol / -14,53522 kJ/mol



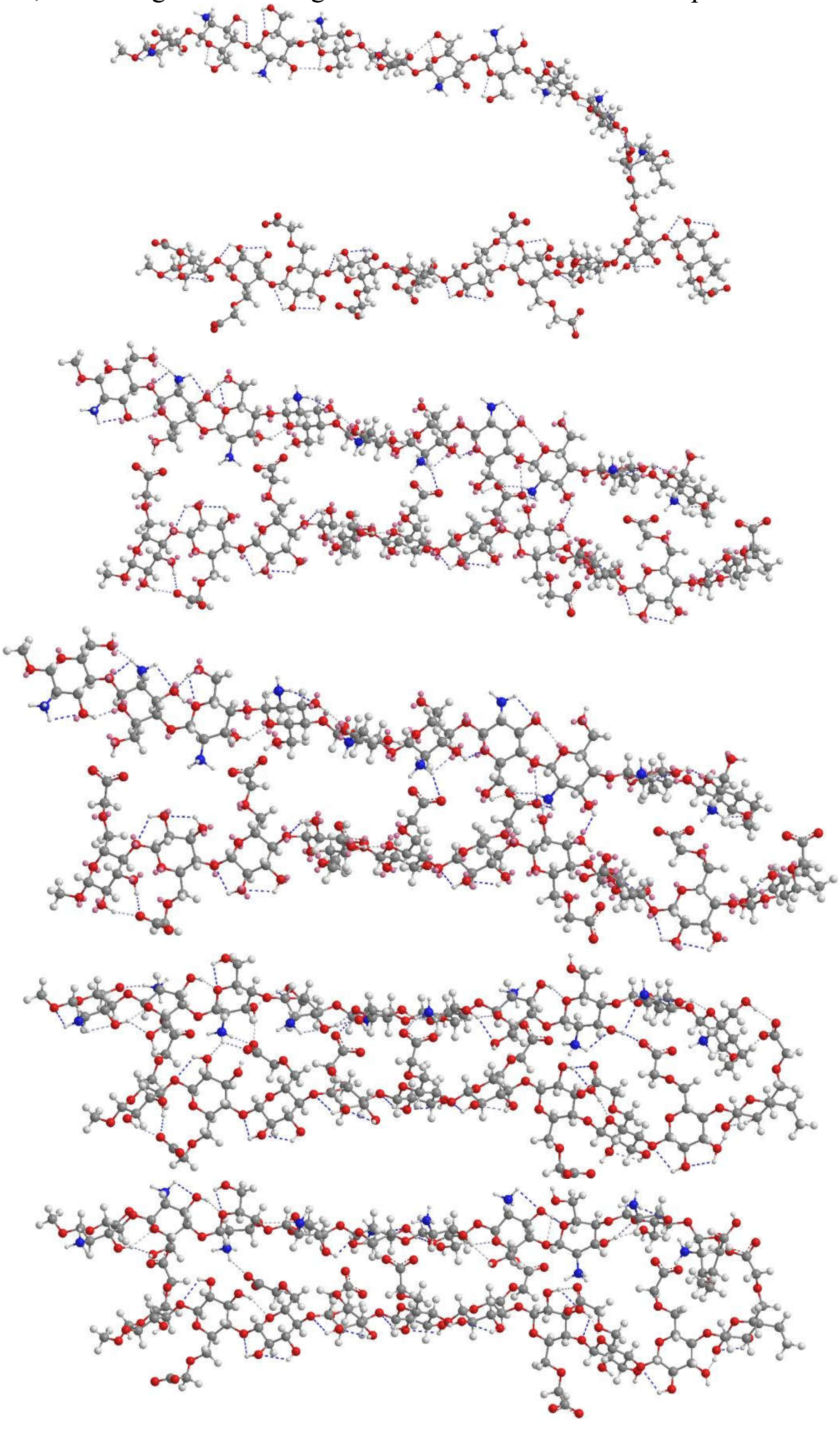
Interaction of a chain of 10 chitosan units containing 5 protonated and 5 non-protonated amino groups with a chain of 10 Na-CMC units. Iteration energy = -2681 kcal/mol / -11,2173 kJ/mol



Interaction of a chain of 10 units of chitosan containing only protonated amino groups with a chain of 10 units of Na-CMC. Iteration 1000: energy = -2129 kcal/mol / -8,907736 кJ/mol

Figure 1. Models of the interaction of chitosan with Na-CMC

The sequence of interaction of the chitosan polycation chain with Na-CMC during the formation of their polyelectrolyte complex was modeled (Figure 10). It is shown that the chains approach quickly in time with the formation of an electrostatic interaction between the polycation and the polyanion, the stability of the chitosan-CMC polyelectrolyte complex is determined by the number of interactions between them, and, as a result, the configuration change of the chains into a more compact structure:



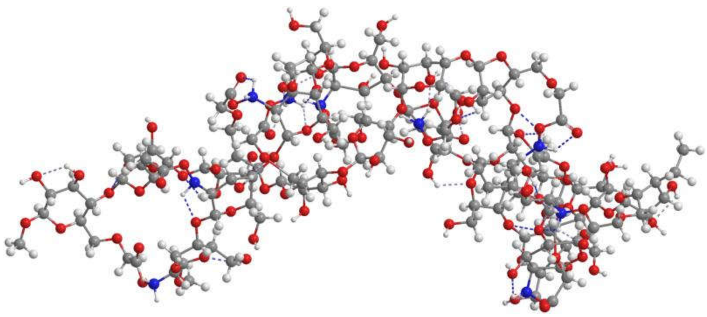


Figure 1. The sequence of interaction of chitosan with Na-CMC during the formation of a polyelectrolyte complex and the structure of the complex when all amino groups of chitosan interact with –COO-groups of CMC

This mechanism of formation of the polyelectrolyte complex, revealed by molecular dynamics modeling, is consistent with the experimental data that the polyelectrolyte complexes of chitosan–CMC are formed due to the electrostatic interaction between the charged -$^{+}NH_3$ groups and the -COO− groups of CMC, i.e. This process is affected by both the pH of the solution and the degree of deacetylation of chitosan.

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АДСОРБЦИОННЫЕ СВОЙСТВА ГИБРИДНЫХ НАНОКОМПОЗИЦИЙ ХИТОЗАН-КРЕМНЕЗЕМ С ВОДОЙ

Акбаров Х.И., Яркулов А.Ю.

Национальный университет Узбекистана

Хитозан - природный биополимер, обладающий рядом уникальных свойств, таких как высокая реакционная способность, устойчивость к радиации, большая сорбционная емкость и селективность по отношению к переходным и тяжелым металлам, хорошая адгезия, биосовместимость с живыми тканями, биодеградируемость, биоинертность. В работах последних лет опубликованы данные о создании на основе хитозана органо-неорганических материалов, состоящих из органической (хитозановой) и неорганической фаз (фосфат или карбонат кальция, оксиды циркония, алюминия, олова, титана и кремния), одна из которых имеет нанометровые размеры. Получение таких гибридных материалов с нанометровыми фазами-альтернативный путь улучшения и модификации свойств полимеров. Одним из путей получения органо-неорганических композитов на основе хитозана является золь-гель-метод, который заключается в гидролизе и поликонденсации различных алкоксисиланов в хитозановой матрице с формированием неорганической фазы оксида кремния. Размеры образующихся в результате этого процесса частиц (SiO_2) можно регулировать, варьируя тип алкоксисилана, соотношение вода:алкоксисилан, природу органических растворителей, pH среды, тип и количество катализатора, температуру синтеза [1].

Изотермы адсорбции воды на хитозан-кремнеземных гибридных нанокомпозиционных материалах в полулогарифмических координатах представлена на рис. Изотерма адсорбции воды на гибридных хитозан-кремнеземных нанокомпозиционных материалах описывается вогнутой кривой