Electronic Structure and Transport Properties of Polypeptide: Polyglycine Chain with Hydrated Side Group

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A calculation on a model compound is performed to test the Brillouin mechanism for the transport properties of proteins.

Very recently [1, 2] we have discussed the electronic structure and transport properties of a model protein compound (polyglycine). The main conclusions are: the forbidden band gap of polyglycine indicates absence of intrinsic semiconduction, and holes can much more probably be considered as conventional delocalized charge carriers than electrons. Many years ago Brillouin [3] proposed a model for explaining the conductivity in proteins. According to this model the conduction takes place along the main polypeptide backbone while the residues (side chains) serve as a source of impurity levels in the forbidden band. The aim of this note is to present results obtained on such a model. We treated a polyglycine chain where a hydrated group $(HCOO)^-$ attached to the main chain serves as an impurity whose energy levels fill up the space between the highest occupied and the lowest vacant electron zones.

The method we have used to deduce the electronic structure and transport properties are given in Ref. [1, 2]. The hydrated group was placed at the NH group of the main chain. The distance between these two groups (connected by hydrogen bond) was optimized in separate calculations on a small cluster system.

The energy gap of hydrated polyglycine (11.9 eV) is much lower than in the polyglycine chain (16.5 eV). Even more dramatic are the changes in the mean free path and mobility of conduction for electrons and holes. The mean free paths are 11.46 Å for electrons and 0.99 Å for holes. The corresponding quantities for polyglycine are 0.36 Å and 1 Å, respectively.

The mobilities for electrons and holes are much larger than in polyglycine. These values are 144.6 cm^2/Vs for electrons and 4.0 cm^2/Vs for holes while the corresponding values for polyglycine are 1.4 cm^2/Vs and 6.1 cm^2/Vs.

The main conclusion of this study is: while in polyglycine holes can probably be considered as the charge carriers the situation is drastically changed when a hydrated group is attached to the chain. The mean free path and the mobility of electrons are much larger than of holes. Electrons can now be considered as conventional delocalized charge carriers in protein models perturbed by a hydrated group. In this note we treat only the conventional semiconduction mechanism (deformation potential approach [1]). Other mechanisms are excluded from our discussion.

[1] M. Kertesz, J. Koller, and A. Ažman, Nature London **266**, 278 (1977).
[2] M. Kertesz, J. Koller, and A. Ažman, Phys. Rev. **B** (in press).
[3] L. Brillouin, Horizons in Biochemistry, Eds. M. Kasha and B. Pullman, Academic Press, New York 1962, p. 295.