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Investigation of physical properties of diphenylalanine peptide nanotubes having different chirality

V.S. Bystrov[1], S.A. Kopyl[2], A.L. Kholkin[2], O.A. Zhulyabina[3], V.A. Tverdislov[3]

[1]*Insitiute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, 142290 Pushchino, Moscow region, Russia*
vsbys@mail.ru

[2]*Department of Physics / CICECO−Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal*

[3]*Physical Faculty, Lomonosov Moscow State University, 119991, Moscow, Russia*

The primary structure of all amino acids exists in 2 different chiralities: L (left) and D (right) [1]. However, in biological nature almost all amino acids are L. This choice is due to evolution process, but its reasons are not enough clear yet. To find some physical sources of such difference the investigation of 2 type of diphenylalanine (FF) peptide nanotubes (PNT), based on L-FF and D-FF, was performed. Both types of PNT were fabricated by standard method and their physical properties (X-ray structural data, optical dichroism, polarization, and piezoelectric response, etc.) were studied.

Computational modeling of both structures was carried out to, using HyperChem software as in our previous studies [2, 3]. We considered two main conformations of initial phenylalanine (F) amino acid molecules (beta-sheet (β) and alfa-helix (α)) in both chiral isomers L and D forms. For all FF PNT we used zwitterion molecular forms and considered our standard 2-ring model consisting from 6 FF in each ring, forming hexagonal structure. Optimized structures show that L-chiral PNT have more strong dipole moment and polarization in both conformations (0.023 C/m^2 for α and 0.05 C/m^2 for β) as compared with D-chiral PNT (0.0073 C/m^2 for α and 0.016 C/m^2 for β). These results give evidence for L-isomers, which are more stable and have higher electric coupling than D-chiral form (because it has third times higher dipole moments), that may be very important for the evolution process. See details in Fig. 1, 2.

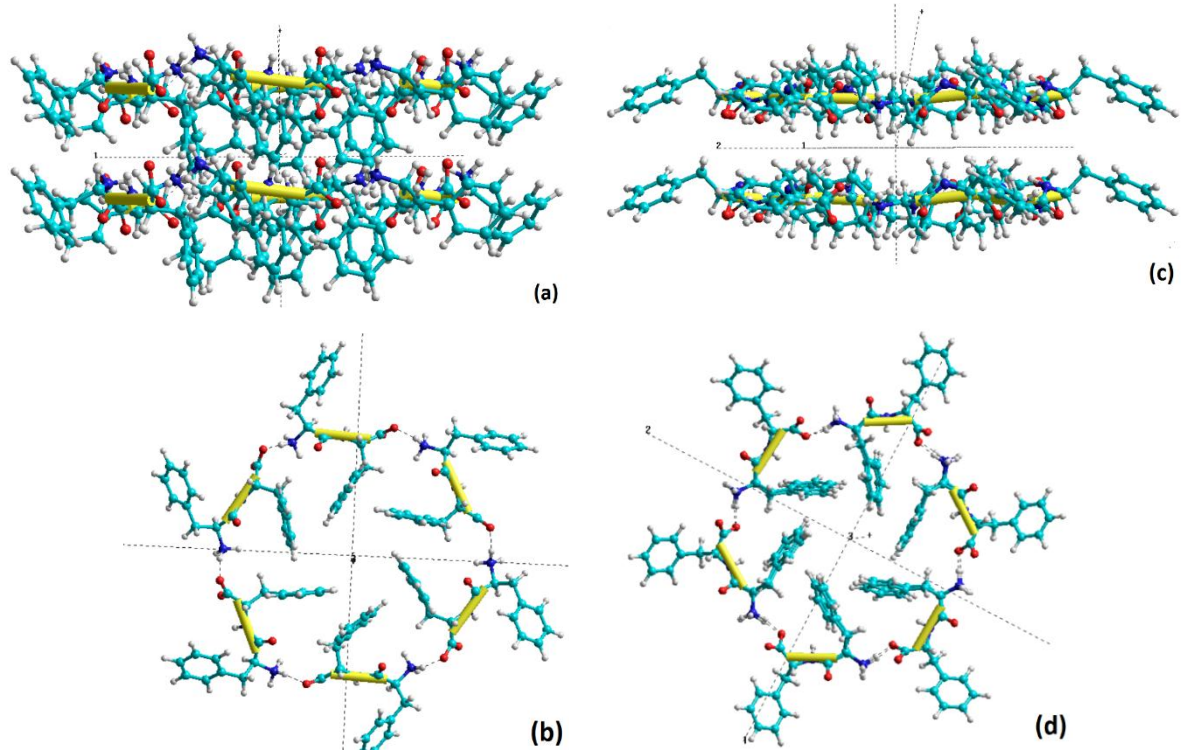

Figure 1. Molecular models of 2 ring FF PNT in β-sheet conformation: a) L-chiral isomer in Y-plane view, b) L-chiral isomer in Z-plane view, c) D-isomer in Y view, d) D-isomer in Z-plane.

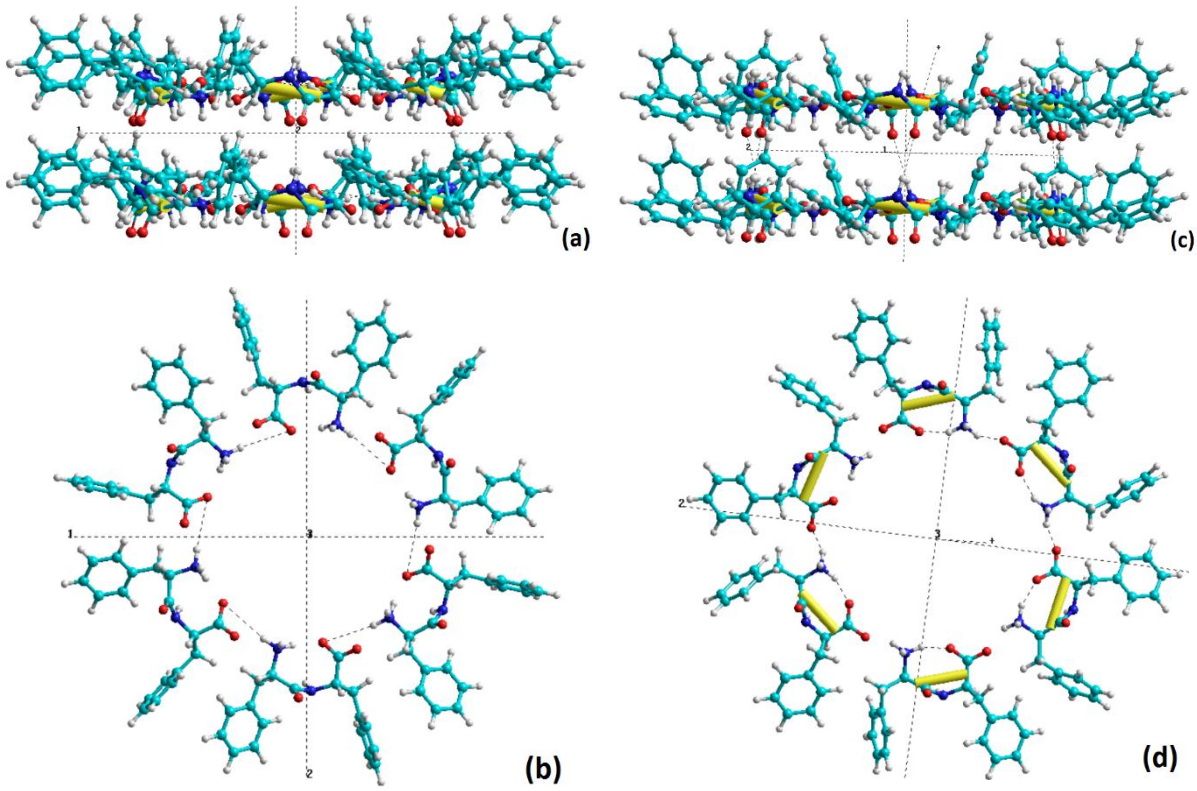

Figure 2. Molecular models of 2 ring FF PNT in helix conformation: a) L-chiral isomer in Y-plane view, b) L-chiral isomer in Z-plane view, c) D-isomer in Y view, d) D-isomer in Z-plane.

These developed models will be used for further studies to investigate the inclusions of the hexagonal ice or water molecular units inside the FF PNT as observed in the several experimental conditions. One of the main structural differences of these FF PNT is that in the case of α-helix conformation inside PNT space is the most empty and, therefore, it is able to take more water molecules.

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3. V.S. Bystrov, E. Paramonova, I. Bdikin, S. Kopyl, A. Heredia, R.Pullar, A. Kholkin. *Ferroelectrics*, **440** (01), 3 (2012).