Water adsorption and polar properties of self-assembled diphenylalanine nanotubes

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Self-assembled micro- and nanotubes of diphenylalanine dipeptide (H-Phe-Phe-OH, FF) represent promising functional biomaterial for new medical and energy harvesting devices [1] due to its outstanding piezoelectric [1, 2], pyroelectric [3] and mechanical [4] properties. After the self-assembly in aqueous solution water molecules remain captured inside the nanochannels, stabilize its structure [5] and modify physical properties. Here we studied water adsorption in FF nanochannels, its structure and polar properties.

Room temperature nitrogen and water adsorption measurements showed that the specific surface area of FF nanotubes is comparable with that of polymers of intrinsic microporosity, several kinds of metal-organic frameworks and porous carbons. Single-crystal X-ray diffraction and computer modeling revealed the reconstruction of the bound water layer at low temperatures, whereas the peptide shell remains almost the same. Temperature of this reconstruction corresponds to a phase transition observed recently at 230 K by dielectric measurements [6]. Ab-initio calculations showed that all analyzed water structures are polar, and the direction and values of their dipole moments were obtained. For all temperatures the dipole moment is mainly oriented along the nanotube’s axis and is opposite to the dipole moment of the peptide shell, thus reducing the total polarization of the nanotube. However, the direct piezoelectric measurements demonstrated non-monotonous decrease of the piezoelectric coefficient with water removing. The origin of this contradiction is not clear yet.

Experimental part of this work was performed within the scope of the project CICECO-Aveiro Institute of Materials, FCT Ref. UID/CTM/50011/2019, financed by national funds through the FCT/MCTES. Theoretical part of the work was supported by Russian Science Foundation (Grant No. 18-72-00052). S.K., P.Z. and A.K. are grateful to FCT project PTDC/CTM-CSTM/31679/2017. P.Z. is grateful to FCT project PTDC/QEQ-QAN/6373/2014. S.K and A.K are grateful to joint Portugal-Turkey project (TUBITAK/0006/2014).