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Charge Transport in Biological Molecules

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Abstract : The focus of this work is on the numerical investigation of the charge transport properties of the de novo-designed alpha3 polypeptide, as well as in its variants, all of them probed by gene engineering. The theoretical framework makes use of a tight-binding model Hamiltonian, together with ab-initio calculations within quantum chemistry simulation. The alpha3 polypeptide is a 21-residue with three repeats of the seven-residue amino acid sequence Leu-Glu-Thr-Leu-Ala-Lys-Ala, forming an alpha–helical bundle structure. Its variants are obtained by Ala→Gln substitution at the e (5th) and g (7th) position, respectively, of the alpha3 polypeptide amino acid sequence. Using transmission electron microscopy and atomic force microscopy, it was observed that the alpha3 polypeptide and one of its variant do have the ability to form fibrous assemblies, while the other does not. Our main aim is to investigate whether or not the biased alpha3 polypeptide and its variants can be also identified by quantum charge transport measurements through current-voltage (IxV) curves as a pattern to characterize their fibrous assemblies. It was observed that each peptide has a characteristic current pattern, which may be distinguished by charge transport measurements, suggesting that it might be a useful tool for the development of biosensors.

Keywords : charge transport properties, electronic transmittance, current-voltage characteristics, biological sensor
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