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Electronic and Transport Properties of Quasi-1D Wires of Biological Molecules BJÖRN OETZEL, LARS MATTHES, FALK TANDETZKY, FRANK ORTMANN, FRIEDHELM BECHSTEDT, KARSTEN HANNEWALD, ETSF and IFTO, Friedrich-Schiller-University Jena, Germany — In the search for organic materials with good charge-transport properties, artificial stacks of biological molecules are considered attractive candidates [1,2]. In this spirit, we present ab-initio DFT calculations of the structural, electronic, and quantum-transport properties of quasi-1D wires based on guanine and eumelanin molecules [3]. Hereby, a special focus is put on the results for the electronic bandwidths and the consequences for potential applications.

[1] R. di Felice et al., Phys. Rev. B 65, 045104 (2001)
[2] P. Meredith et al., Pigment Cell Res. 19, 572 (2006)
[3] B. Oetzel et al. (unpublished)

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