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.