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Molecular Electronics with Peptide Nanotubes: Calculation of Conventional and Complex Band Structure RIBEKA TAKAHASHI, HAO WANG, JAMES LEWIS, Brigham Young University — We have studied the electronic structure of three peptide nanotubes which have been proposed as a potential nanowire. We choose nanotubes which have different sequences of amino-acid residue: (L-Gln, D-Ala)$_4$, (L-Gln, D-Leu)$_4$, and (L-Gln, D-Phe)$_4$. We calculated the conventional band structure and the complex band structure of the peptide nanotubes. Our study of the conventional band structure shows that the peptide nanotubes generally have large band gaps (4 eV); however, the band gap decreases due to the presence of aromatic rings in the side chain of peptide nanotubes. Our study of the complex band structure predicts that the molecular tunneling conductivity of peptide nanotubes is small.

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