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A Novel Technique for Generating a Band Diagonal Matrix in Tight-Binding DNA Analysis DALE IGRAM, ERIC HEDIN, YONG JOE, Department of Physics and Astrnomy, Ball State University — There exist numerous selection sequence techniques for creating a coupling integral matrix for the calculation of transmission of an electron through a DNA molecule. However, these techniques typically create a matrix which requires a significant amount of computer time and memory, especially for large DNA models. Presented here is a novel technique that generates a band diagonal coupling integral matrix which reduces the computer time and memory required for the calculations. To illustrate the benefits, Poly(G)-Poly(C) 4-channel DNA models for 3-basepairs, 5-basepairs, and 7-basepairs are used to compare the CPU calculation time of the different models. A graphical representation will reveal the benefit of using this novel technique.

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