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Molecular Assembly for Hybrid Electronics BANSAL JUHI, Dept of Materials Science and Engg, SUNY at Stony Brook, DILIP GERSAPPE, Dept of Materials Science and Engg, SUNY at Stony Brook — The process of forming molecular switches depends critically on the ability to bridge the nanoscale gap between electrodes. The probability that a molecule will bridge this gap depends on a number of factors such as the length of the molecule, its conformational rigidity and the solvent under which the deposition is performed. We use the Rotational Isomeric Scheme to model the rigidity of the molecule and predict conditions under which molecules will bridge the gap between the two electrodes. In our simulations we vary the aspect size of the electrodes, the distance between them and the the size of the molecule. Finally, we use the results of our RIS model to feed into a Monte Carlo simulation that predicts the connectedness of a series of nanowires. The Monte Carlo simulation accounts for the inherenet fluctuations that can occur in the electrode spacing and the aspect ratio of the electrodes.

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