

Electronic Supplementary Information for: Thermal-induced Charge Carrier Population Control on Graphene Nanoribbons[†]

T. S. A. Cassiano¹, G. M. e Silva^{1,*}, and P. H. de Oliveira Neto^{1,2}

¹ *University of Brasília, Institute of Physics, 70.910-900, Brasília, Brazil*

² *International Center of Physics, University of Brasília, 70919-970, Brazil*
*magela@unb.br**

1 Statistical Stability

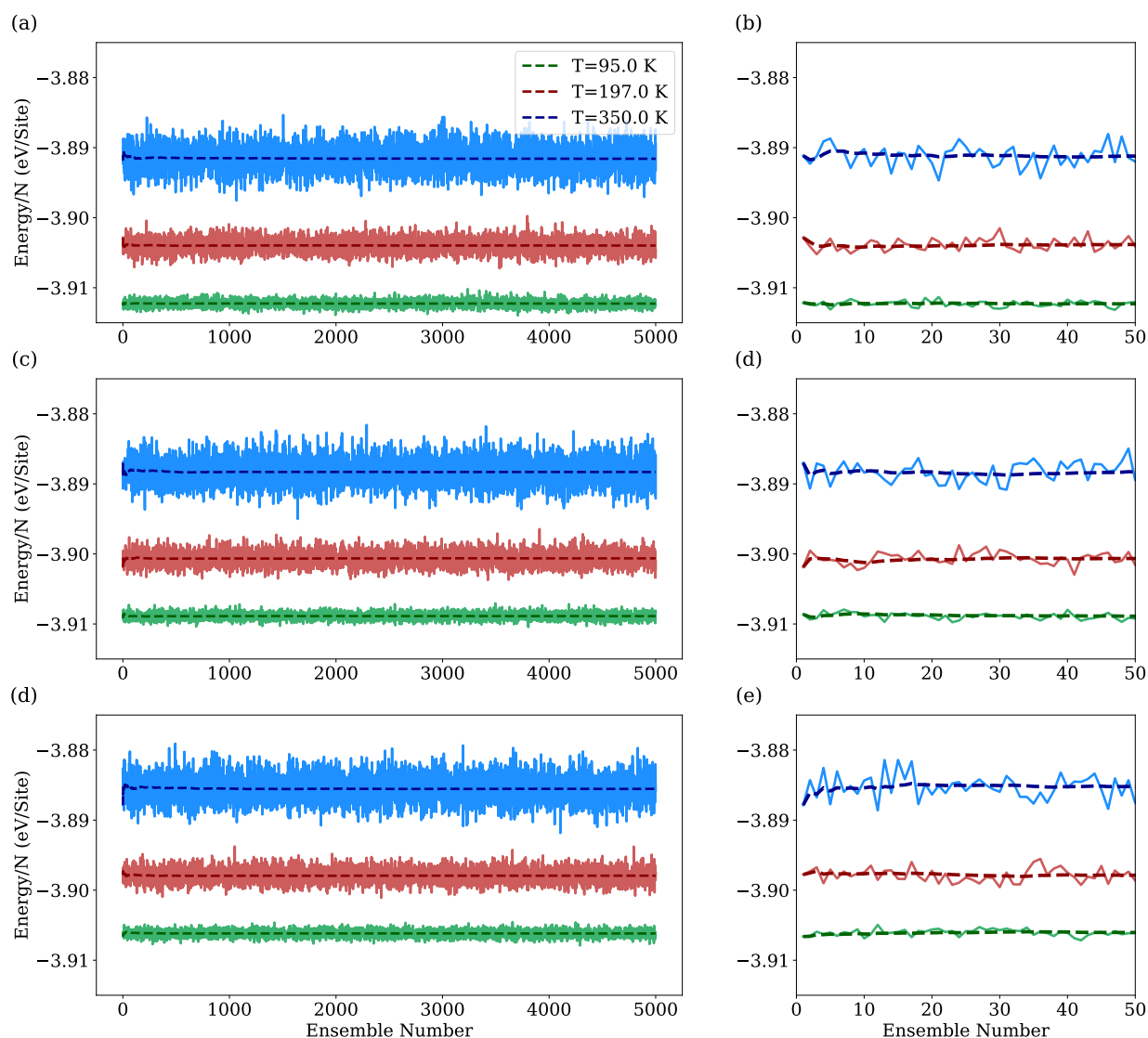


Figure S1: Verification of statistical stability when using ensemble of 5000 elements. (a), (c), and (d) present the total energy (divided by the number of sites) for the 4AGNR in the neutral, polaron and bipolaron states. The colors indicate the ensemble's temperature. The solid lines are the corresponding energies for each ensemble element. The dashed lines are their cumulative mean values. (b), (d), and (e) are zoomed versions of the (a), (c), and (d).

2 Average of Ensemble Members

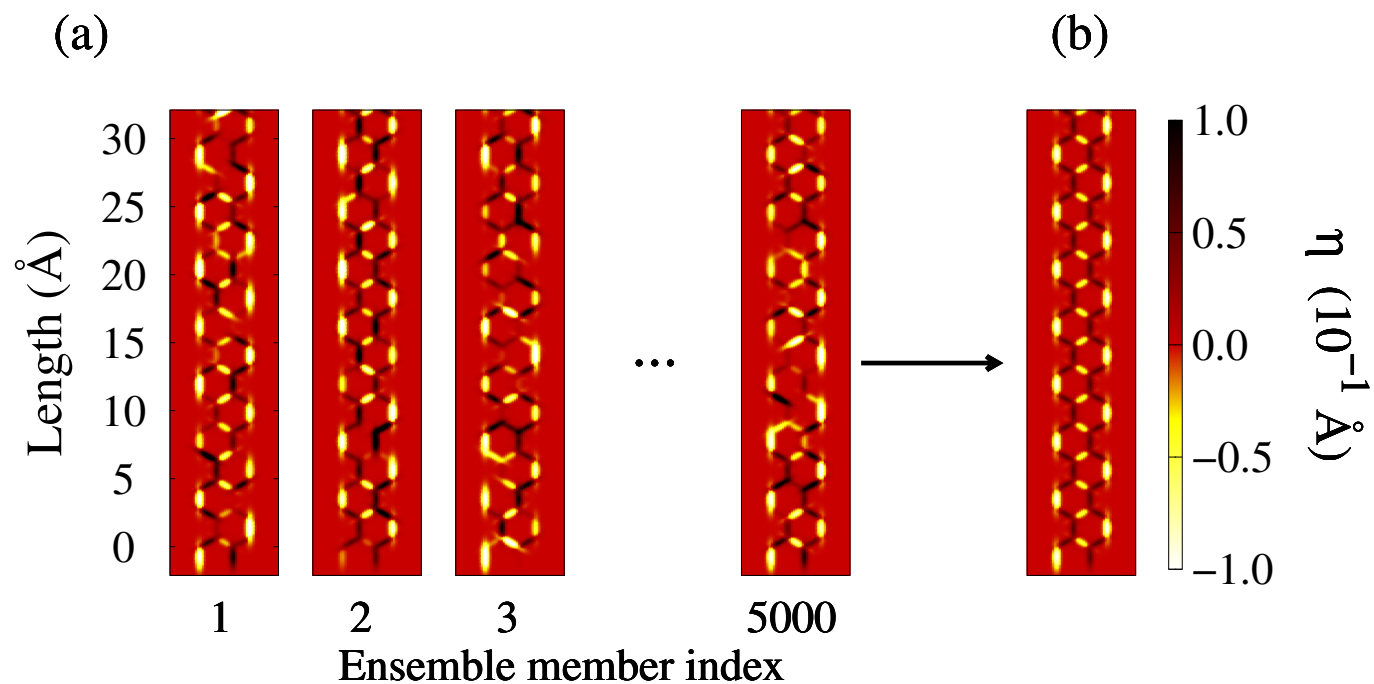


Figure S2: Representation of a geometry ensemble of 4AGNR for $T = 294$ K. The average of all 5000 ensemble members, represented in (a), result in the profile shown in (b). The heatmap colors follow the same convention defined in Figure 2.

3 Lattice Distortion Profile

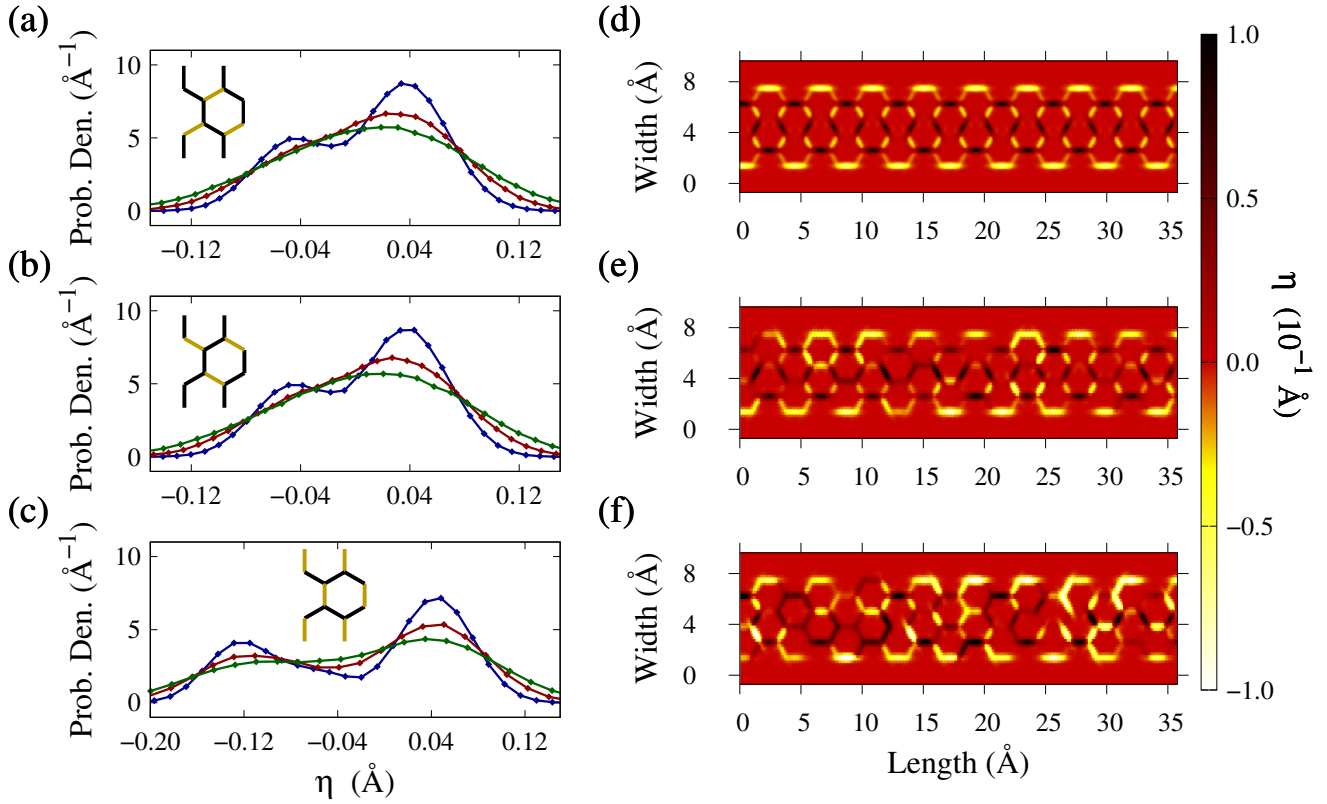


Figure S3: Bond deformations in the presence of thermal effects in neutral 6AGNR. (a), (b) and (c) are, respectively, the deformation distributions for the trans (/), cis (\) and vertical (|) bonds. At each plot, a GNR slice illustration is placed to exhibit, in yellow, the corresponding bond type. The blue, red, and green curves correspond to $T = 95, 197$, and 350 K. In addition, (d), (e), and (f) are the bond deformation heatmaps for $T = 0, 95$, and 350 K. Dark colors refer to expanded bonds, while light tones indicate contraction.

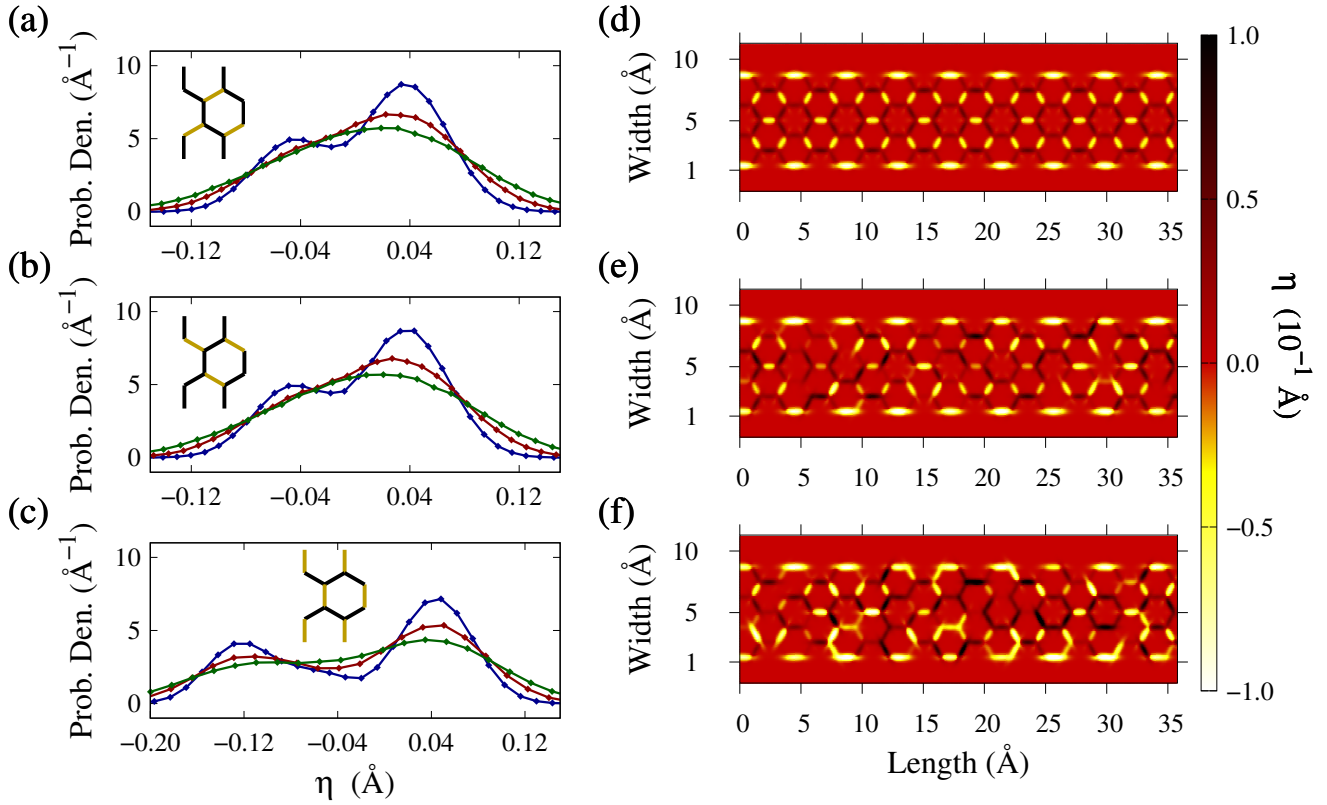


Figure S4: Bond deformations in the presence of thermal effects in neutral 7AGNR. (a), (b) and (c) are, respectively, the deformation distributions for the trans (/), cis (\) and vertical (|) bonds. At each plot, a GNR slice illustration is placed to exhibit, in yellow, the corresponding bond type. The blue, red, and green curves correspond to $T = 95$, 197, and 350 K. In addition, (d), (e), and (f) are the bond deformation heatmaps for $T = 0$, 95, and 350 K. Dark colors refer to expanded bonds, while light tones indicate contraction.

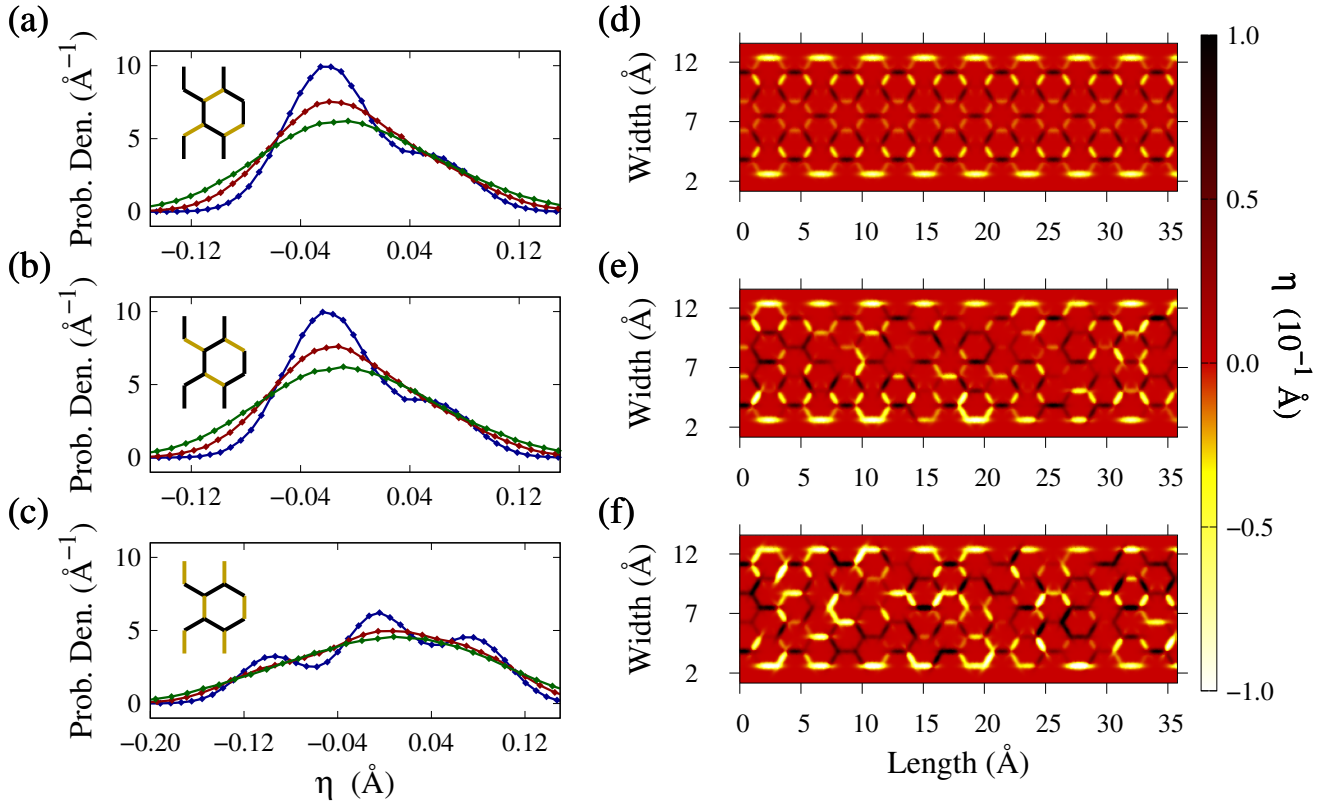


Figure S5: Bond deformations in the presence of thermal effects in neutral 9AGNR. (a), (b) and (c) are, respectively, the deformation distributions for the trans (/), cis (\) and vertical (|) bonds. At each plot, a GNR slice illustration is placed to exhibit, in yellow, the corresponding bond type. The blue, red, and green curves correspond to $T = 95$, 197 , and 350 K. In addition, (d), (e), and (f) are the bond deformation heatmaps for $T = 0$, 95 , and 350 K. Dark colors refer to expanded bonds, while light tones indicate contraction.

4 Formation Energy Distributions

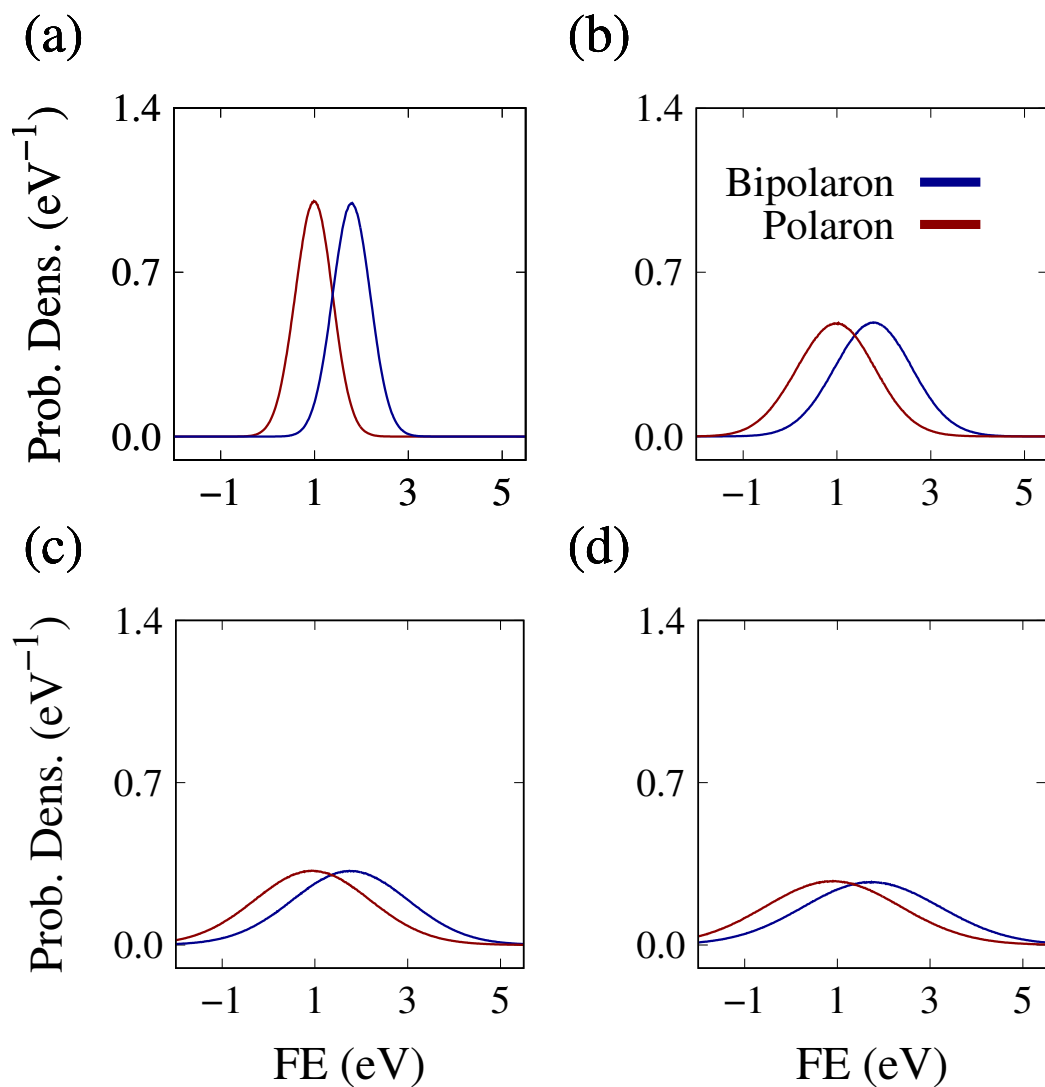


Figure S6: 6AGNR Probability density distribution of the polaron (red) and bipolaron (blue) formation energies. (a), (b), (c), and (d) refer to, respectively, $T = 95, 197, 299$, and 350 K cases.

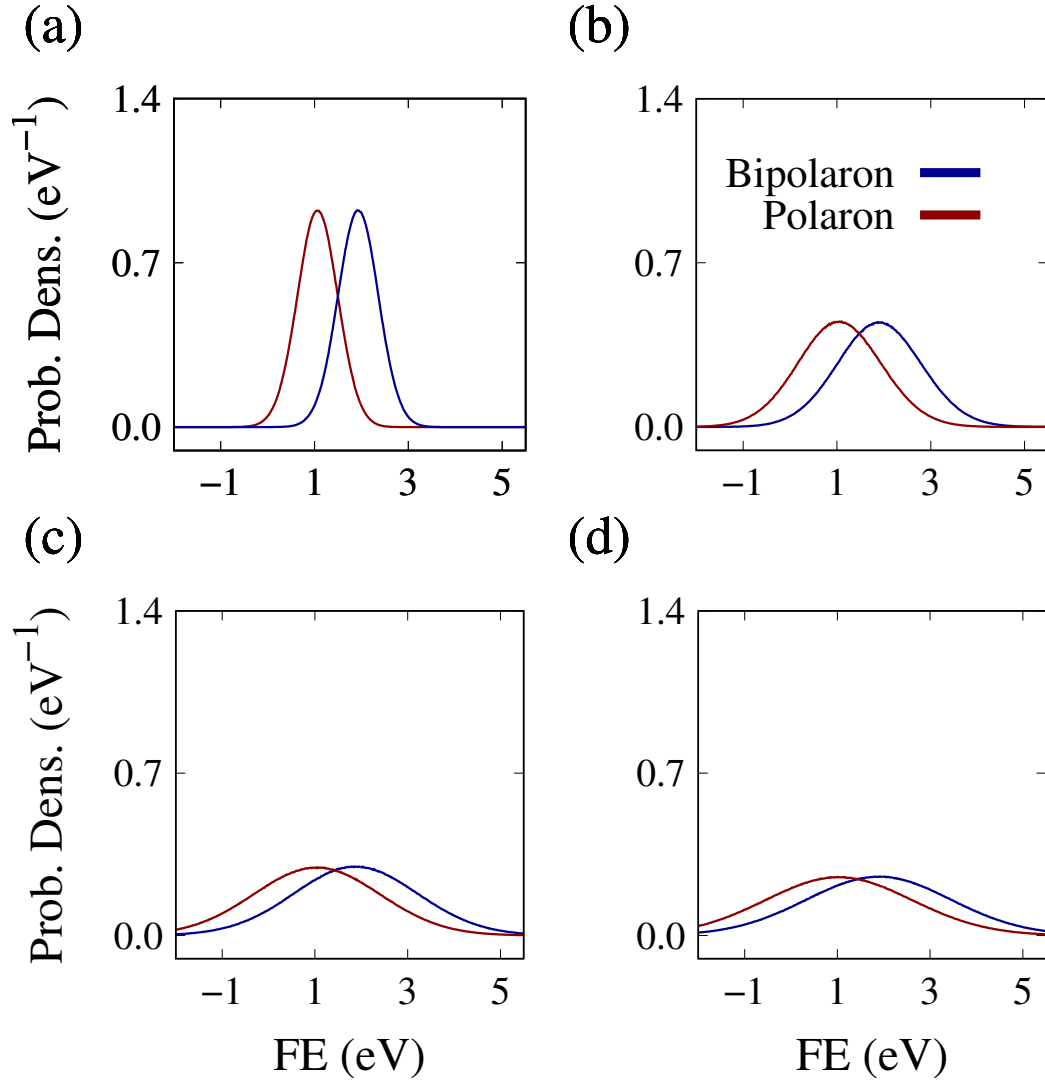


Figure S7: 7AGNR Probability density distribution of the polaron (red) and bipolaron (blue) formation energies. (a), (b), (c), and (d) refer to, respectively, $T = 95, 197, 299$, and 350 K cases.

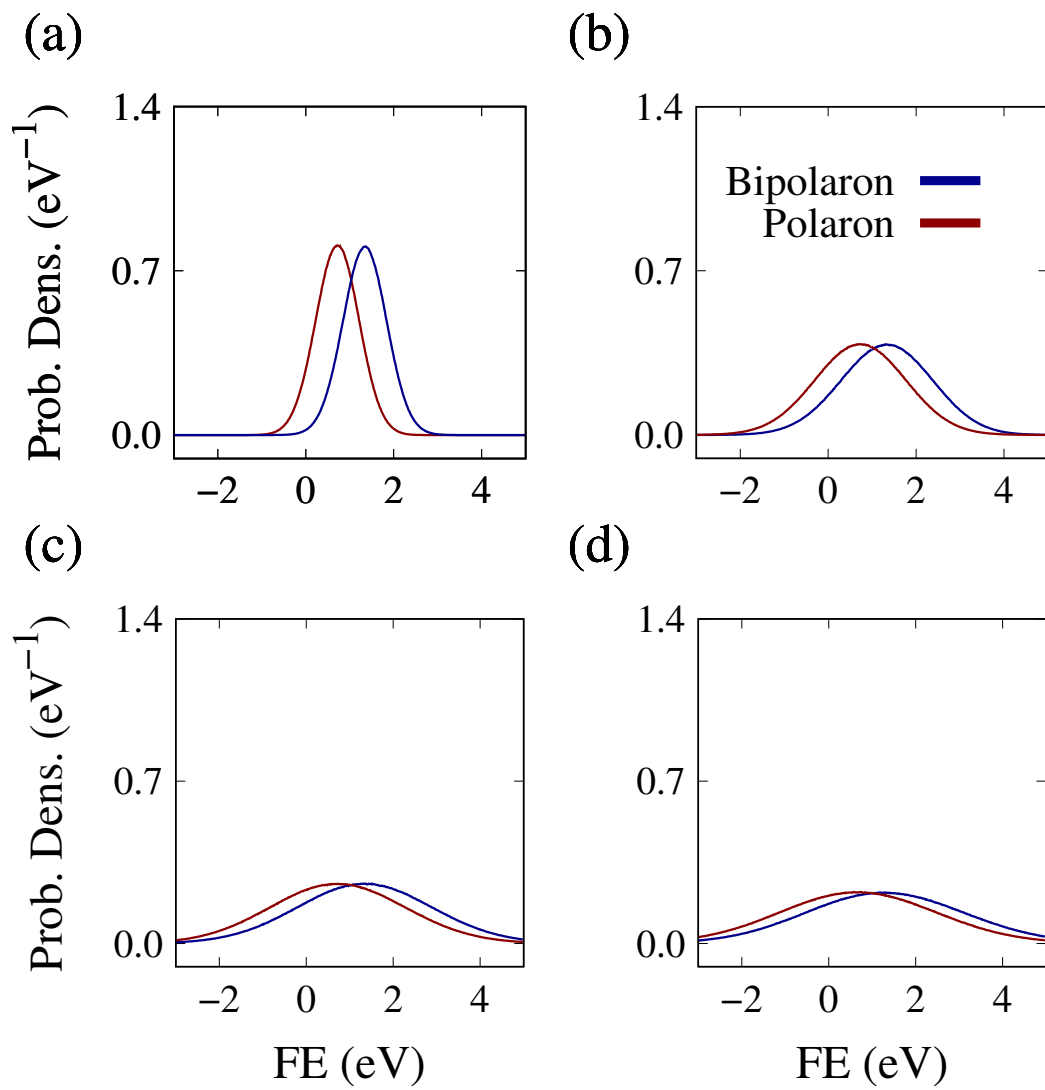


Figure S8: 9AGNR Probability density distribution of the polaron (red) and bipolaron (blue) formation energies. (a), (b), (c), and (d) refer to, respectively, $T = 95, 197, 299$, and 350 K cases.